CRYSTALS OF THE *ESCHERICHIA COLI* MEMBRANE-ASSOCIATED GLYCOSYLTRANSFERASE (MurG) PROTEIN, ATOMIC COORDINATES AND THREE DIMENSIONAL STRUCTURES THEREOF, ATOMIC COORDINATES AND THREE DIMENSIONAL STRUCTURES OF BINDING DOMAINS THEREOF, IMAGES THEREOF, AND METHODS OF CRYSTALLIZING MurG PROTEINS, MODELS OF UDP-GLYCOSYLTRANSFERASES, MurG PROTEINS AND BINDING SITES, METHODS OF MAKING MODELS, METHODS OF USING MODELS OF MURG, COMPOUNDS THAT BIND, INHIBIT OR STIMULATE MURG PROTEINS, AND THERAPEUTIC COMPOSITIONS THEREOF

FIELD OF THE INVENTION

The present invention relates to crystals of the *Escherichia coli* MurG, a membrane-associated UDP-glycosyltransferase involved in peptidoglycan biosynthesis. The present invention also relates to three-dimensional atomic coordinates of the MurG protein, three-dimensional structures of the protein, and images thereof. The present invention also relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone of the MurG protein and images thereof. The present invention further relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone and conserved amino acid residue sidechains of the MurG protein and images thereof. The present invention further relates to three-dimensional atomic coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, three-dimensional structures of the binding domains, and images thereof. The present invention also relates to computer readable media encoded with sets of the three dimensional coordinates of the *E. coli* MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and the conserved amino acid residue sidechains of the MurG protein, the donor nucleotide binding site, the acceptor binding site, and the membrane association site. The present invention relates to methods of crystallizing MurG proteins.

The present invention relates to models of three dimensional structures of UDP-glycosyltransferases and, in particular, MurG proteins, based on the three dimensional structure of crystals of the *Escherichia coli* MurG. The present invention also relates to models of the three dimensional structures of the α-carbon backbone of UDP-glycosyltransferases and MurG proteins. The present invention further relates to models of the three dimensional structure of the α-carbon backbone and conserved amino acid residue sidechains of gUDP-glycosyltransferases, in particular, MurG proteins. The present invention further relates to models of the three-dimensional structures of donor nucleotide binding sites, acceptor binding sites, and membrane association sites of UDP-glycosyltransferases, in particular, MurG proteins. The present invention also relates to methods of drug design using models of this invention. The present invention further relates to compounds identified using models of the present invention that bind, inhibit or stimulate UDP-glycosyltransferases or MurG proteins. The present invention relates to compositions comprising compounds identified using the models of this invention for therapeutic or diagnositic uses. Also, the present invention relates to methods of making models of the present invention.

BACKGROUND OF THE INVENTION

The increasing frequency of resistance to existing antibiotics represents a serious public health threat. Structural and mechanistic information on essential bacterial enzymes could lead to the development of antibiotics that are active against resistant microorganisms. Both gram positive and gram negative bacterial cells are surrounded by a cross-linked carbohydrate polymer, peptidoglycan, which protects them from rupturing under high osmotic pressures. Many of the best antibiotics function by inhibiting peptidoglycan synthesis, which ultimately causes cell lysis. In recent years, intense effort has been focused on determining the structures of the enzymes that synthesize peptidoglycan. Structures of several of the early enzymes in the biosynthetic pathway have been reported (Benson *et al.*, 1995; Bertrand *et al.*, 1997; Fan *et al.*, 1994; Skarzynski *et al.*, 1996); however, the later enzymes have proven more difficult to study because both they and their substrates are membrane-associated.

MurG is the last enzyme involved in the intracellular phase of peptidoglycan synthesis (Bugg & Walsh, 1993). It catalyzes the transfer of N-acetyl glucosamine

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(NAG) from UDP to the C4 hydroxyl of a lipid-linked N-acetylmuramoyl pentapeptide (NAM) to form a ?-linked NAG-NAM disaccharide that is transported across the cell membrane where it is polymerized and cross-linked (Fig. 1). In bacterial cells MurG associates with the cytoplasmic surface of the membrane (Bupp & van Heijenoort, 1993). However, we have found that *E. coli* MurG can be solubilized at high concentrations in active form (Ha *et al.*, 1999).

The elucidation of the protein structure of a MurG protein is of importance in the identification and formulation of anti-bacterial agents. Until the discovery of the present invention, the structure and resulting mechanism by which MurG functions was not known. Thus, despite the important role of MurG in peptidoglycan synthesis, development of useful agents for treatment or diagnosis of disease was hindered by lack of structural information of the protein.

In order to obtain structural information on a MurG protein, it is important to have purified, active enzyme. The demonstration of activity requires a suitable assay, which in turn requires access to the natural substrates or analogues thereof. The study of MurG was hampered by difficulties obtaining and handling the lipid-linked NAM substrate (commonly known as Lipid I). This problem was overcome by Walker and coworkers, who developed a synthetic route to a set of substrate analogues of Lipid I that were shown to function as glycosyl acceptors in a glycosyl transfer reaction catalyzed by MurG. Some of these substrate analogues are freely water soluble, making it possible to monitor the activity of purified *E. coli* MurG in buffer in the absence of natural or artificial membranes or detergents.

The linear nucleic acid and amino acid sequences of *E. coli* MurG were reported in 1992. Subsequently, the nucleic acid and amino acid sequence of *B. subtilus* MurG was reported. Since then, many bacterial genomes have been sequenced and the information has been deposited in databases. Information based only on linear sequences, however, cannot accurately predict the three-dimensional structure of the protein and its functional domains.

Therefore, there is a need in the art to elucidate the three-dimensional structure of a MurG protein. One three dimensional structure of a MurG protein can be used to construct models of other MurG proteins and to facilitate the structure determination of crystalline forms of other MurG proteins. Structures and models of MurG proteins can

also be used to design proteins containing only the donor binding site or the acceptor binding site. These proteins can be used in assays, including NMR-based assays, to identify -- or characterize the mode of binding of -- ligands that bind in or near the vicinity of the substrates. These ligands or compounds can then be used as leads for the design of inhibitors that have therapeutic activity. Structures and models of MurG proteins can also be used in computer-based drug design.

SUMMARY OF THE INVENTION

The present invention relates to crystalline *Escherichia coli* MurG protein. Obtaining such crystals is an unexpected result. It is well known in the protein crystallographic art that obtaining crystals of quality sufficient for determining the structure of a protein is unpredictable. In particular, obtaining crystals of quality sufficient for determining the three-dimensional (3-D) structure of MurG has not been achievable until the crystallization of MurG as disclosed in the present application. As such, determination of the three-dimensional structure of MurG has not been possible until the discovery of the present invention. Additionally, until the discovery of the present invention, derivation of the three-dimensional structure and models of other MurG proteins has not been possible. The present inventors are also the first to define the three-dimensional structure and provide three-dimensional models for drug design for MurG proteins.

Accordingly, one object of the present invention is to provide crystals of sufficient quality to obtain a determination of the three-dimensional atomic coordinates and structures of MurG to high resolution, preferably to the resolution of less than 2.0 angstroms (Å). The present invention also provides methods for producing crystalline MurG protein.

The value of the crystals of *E. coli* MurG protein extends beyond merely being able to obtain such crystals. The knowledge obtained concerning the MurG crystal structure, for example, has been used by the present inventors to define the heretofore unknown tertiary structure of the MurG protein and to identify the location of the glycosyl donor and glycosyl acceptor binding domains, as well as the location of the amino acid residues that are invariant in all MurG proteins. This information can be used to design inhibitors of MurG that have therapeutic utility. The atomic coordinates of *E.*

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coli MurG also are used to model the heretofore unknown tertiary structures of other MurG proteins having substantially related linear amino acid sequences, such as for MurG proteins from other microorganisms. It is anticipated that homology models can be constructed even from amino acid sequences with relatively low homology because the present inventors have identified the location of the invariant amino acid residues in MurG. The relative spatial orientations of such residues is expected to be conserved in all MurG proteins.

Comparison of nucleic acid and amino acid sequences of MurG proteins indicates that the linear amino acid sequences can vary significantly. Homology between MurG proteins from different microorganisms varies from less than 30% to greater than 90%, reflecting the evolutionary relationship between the organisms. The low homology between distantly related MurG homologues is not believed to reflect significantly different folded structures. It is well known that many amino acid sequences are capable of adopting the same general fold. *E. coli* MurG contains an alpha/beta folding pattern, one of the most common folds known in proteins. It is likely that all MurG homologues contain a similar alpha/beta fold despite the differences in the linear amino acid sequences. What gives these proteins their identity is not the general fold, but the specific details − *i.e.*, the presentation of certain amino acids on the folded structure. The present inventors have identified the location in *E. coli* MurG of a set of residues that are invariant in all MurG homologues. It is to be expected that these residues would adopt a similar spatial location with respect to the folded structure in all MurG homologues. Therefore, these invariant residues, which have been selected by evolution as the critical residues for the binding and catalytic function of the protein, provide essential information on the location of the active site and on critical contacts to the substrates/products. They also serve as constraints that make it possible to predict the three-dimensional structures even of distantly related MurG homologues. Thus, knowledge of the three-dimensional structure of the *E. coli* MurG protein has provided a starting point for investigation into the structure of all MurG proteins.

Accordingly, a object of the present invention is to provide information regarding the atomic coordinates and three-dimensional structures of (1) the MurG protein, (2) the α-carbon backbone of the MurG protein, (3) the α-carbon backbone and conserved

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amino acid residues of the MurG protein, (4) the donor nucleotide binding site, (5) the acceptor binding site, and (6) the membrane association site MurG proteins.

It is also an object of this invention to solve the three-dimensional structure of UDP-glycosyltransferases, in particular target MURG proteins, and to determine their structure and/or atomic coordinates. Further, it is an object of this invention to use the structure or atomic coordinates of the *E. coli* MurG crystal to solve the structure of different MURG protein crystals, or a crystal of a mutant protein, homolog or co-complex of MurG.

The present invention relates to models of three dimensional structures of UDP-glycosyltransferases, in particular MurG proteins, based on the atomic coordinates of crystalline *E. coli* MurG protein.

It is a further object of this invention to provide UDP-glycosyltransferase enzyme mutants characterized by one or more different properties as compared with wild-type MURG. These properties include altered surface charge, increased stability to subunit dissociation, altered substrate specificity or higher specific activity. MURG mutants are useful to identify those amino acids that are most important for the enzymatic activity of MURG. This information, in turn, allows the design of improved inhibitors of MURG as compared with peptidic MURG inhibitors.

Another object of the present invention is to provide computer readable mediums encoded with a set of three-dimensional coordinates of the *E. coli* MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and conserved amino acid residues of the MurG protein, and the nucleotide donor binding site, the acceptor binding site, the membrane association site of the MurG protein.

Another embodiment of the present invention provides three-dimensional and two-dimensional computer images of the three dimensional structure of MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and conserved amino acid residues of the MurG protein, and the nucleotide donor binding site, the acceptor binding site, the membrane association site of the MurG protein.

The knowledge of the three dimensional structure of MurG also provides a means for designing proteins that have altered beneficial functions by analyzing the structure and interactions between individual amino acids of the protein. For example, the present inventors have shown that E. coli MurG consists of two domains separated by a cleft.

Noncovalent interactions between the two domains are not extensive. The present inventors have shown that the domains fold independently and can, therefore, be expressed independently either alone or as part of a recombinant protein containing the acceptor binding site from one MurG homologue and the donor binding site from another MurG homologue. It would be expected that the domains of other MurG proteins could also be expressed independently, either alone or as chimaeras with other MurG domains. Independently expressed domains of the protein are useful for discovering ligands that bind to the individual domains.

The knowledge of the three-dimensional structure of *E. coli* MurG protein and models of other MurG proteins also provides a means for designing and producing compounds that regulate, inhibit or antagonize functions of the MurG protein (i.e., structure based drug design). For example, chemical compounds can be designed to block binding of UDP-GlcNAc to a MurG protein using various computer programs and models.

It is also an object of this invention to use the structure coordinates and atomic details of MURG, or its mutants or homologues or co-complexes, to design, evaluate computationally, synthesize and use inhibitors of MURG that avoid the undesirable physical and pharmacologic properties of peptidic MURG inhibitors.

Another embodiment of the present invention is a composition comprising MurG protein in a crystalline form.

Yet another embodiment of the present invention is a method for producing crystals of MurG, comprising combining MurG protein in a suitable buffer with a suitable amount of a reservoir buffer containing a detergent, and inducing crystal formation to produce said MurG crystals.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1. Pathway for peptidoglycan biosynthesis.

Fig. 2. Overall architecture of MurG. **A.** Stereo view of the MurG structure. The N domain is shown in purple; the C domain is shown in green. The figure was generated with the programs MOLSCRIPT (Klaulis, 1991) and RASTER3D (Merrit & Murphy, 1994). **B.** Topology diagram of MurG.

Fig. 3. Identification of critical residues in MurG and related glycosyltransferases. **A.** Sequence alignment of *E. coli* MurG with homologs from seven other bacterial strains, deliberately chosen to represent a disparate group of organisms. The secondary structure of *E. coli* MurG is shown above the sequences. Gaps mapping to the loop regions of *E. coli* MurG suggest that some sequences include other structural elements. Residues highlighted in blue are invariant among the eighteen MurG sequences available. Residues highlighted in yellow are identical in 85% of the eighteen homologs, while in the remaining 15%, only closely related amino acid substitutions are found. Highly conserved residues that do not meet the stringent criteria established for highlighting are shown in the consensus sequence. A consensus motif for UDP-glucuronosyltransferases is also shown. Numbering is with respect to the overexpressed *E. coli* MurG construct, which contains an additional N-terminal methionine. **B.** Mapping of the G loops and other highlighted residues from Fig. 3a in red on the MurG structure. Side chains for highly conserved residues are also shown. **C.** Model for the proposed UDP-binding subdomain found in many UDP-glycosyltransferases based on the *E. coli* MurG structure. Conserved residues in UDP-glucuronosyltransferases are highlighted in red. Side chains are shown for residues that are located near the cleft and may be involved in substrate binding. The glutamate residue is proposed to interact with the ribose sugar. The dotted loop varies in length within the MurG family and in other UDP-sugar transferases, but the N and Q on the following helix are invariant. Note that the UDP-glucuronosyltransferases contain a conserved D preceding the Q, which is not shown on this model.

Fig 4. Structural analysis of the substrate binding pockets in MurG. **A.** Structural comparison between the C-terminal domain of phage T4 ?-glucosyltransferase (left) and the C-terminal domain of *E. coli* MurG (right). The aligned six ?-strands are magenta, the aligned ?-helices are orange, and the other structural elements are blue. In ?-glucosyltransferase, key residues involved in UDP binding are highlighted in yellow. The analogous residues in MurG are also highlighted in yellow. **B.** A close-up view of the proposed donor binding pocket in the MurG C domain with the docked UDP-GlcNAc. Conserved residues in MurG are colored magenta. The carbonyl oxygen of

residue I245 is shown in red, and its backbone nitrogen is shown in blue. C. The surface of *E. coli* MurG. The G loops and other conserved residues in MurG are colored magenta. The proposed membrane binding interface is also highlighted with hydrophobic residues in yellow and positively charged residues in blue.

DEFINITIONS

It is to be noted that the term "a" or "an" entity refers to one or more of that entity; for example, a compound refers to one or more compounds or at least one compound. As such, the terms "a" (or "an"), "one or more", and "at least one" can be used interchangeably herein.

It is also to be noted that the terms "comprising", "including" and "having" can be used interchangeably. Furthermore, a compound "selected from the group consisting of" refers to one or more of the compounds in the list that follows, including mixtures (i.e., combinations) of two or more of the compounds.

According to the present invention, an isolated, or pure, protein, is a protein that has been removed form its natural milieu. As such, "isolated" and "biologically pure" do not necessarily reflect the extent to which the protein has been purified, An isolated protein of the present invention can be obtained from its natural source, can be produced using recombinant DNA technology or can be produced by chemical synthesis.

It is also to be noted that the terms "tertiary" and "three dimensional" can be used interchangeably.

It is also to be noted that reference to a "MurG protein" can also be recited as "MurG" and such terms can be used to refer to the complete MurG protein, a portion of the MurG protein, such as a polypeptide.

The following terms are also used herein:

The term "naturally occurring amino acids" means the L-isomers of the naturally occurring amino acids. The naturally occurring amino acids are glycine, alanine, valine, leucine, isoleucine, serine, methionine, threonine, phenylalanine, tyrosine, tryptophan, cysteine, proline, histidine, aspartic acid, asparagine, glutamic acid, glutamine, .gamma.-carboxyglutamic acid, arginine, ornithine and lysine. Unless specifically indicated, all amino acids referred to in this application are in the L-form.

The term "unnatural amino acids" means amino acids that are not naturally found in proteins. Examples of unnatural amino acids used herein, include racemic mixtures of selenocysteine and selenomethionine. In addition, unnatural amino acids include the D or L forms of nor-leucine, para-nitrophenylalanine, homophenylalanine, para-fluorophenylalanine, 3-amino-p2-benzylpropionic acid, homoarginine, and D-phenylalanine.

The term "positively charged amino acid" includes any naturally occurring or unnatural amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged naturally occurring amino acids are arginine, lysine and histidine.

The term "negatively charged amino acid" includes any naturally occurring or unnatural amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged naturally occurring amino acids are aspartic acid and glutamic acid.

The term "hydrophobic amino acid" means any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of naturally occurring hydrophobic amino acids are alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan and methionine.

The term "hydrophilic amino acid" means any amino acid having an uncharged, polar side chain that is relatively soluble in water. Examples of naturally occurring hydrophilic amino acids are serine, threonine, tyrosine, asparagine, glutamine, and cysteine.

The term "MurG" refers to a UDP-glycosyltransferase that has a two domain strucuture, where each domain contains a set of invariant residues as shown in Figure 3a, including any mutant, homologue or co-complex or any similar enzyme that catalyzes the transfer of N-acetylglucosamine (GlcNAc) from UDP to the C4 hydroxyl of the lipid-linked MurNAc pentapeptide.

The term "mutant" refers to a MurG polypeptide, *i.e.,* a polypeptide displaying the biological activity of a wild-type MurG, characterized by the replacement of at least one amino acid from the wild-type, *E. coli* MURG sequence according to Ikeda, et al., Nucleic Acids Res. 1990, and Mengin-LeCreuix et al., Nucleic Acids Res. 1990. Such a

mutant may be prepared, for example, by expression of MURG cDNA previously altered in its coding sequence by PCR-based mutagenesis method.

MurG mutants may also be generated by site-specific incorporation of unnatural amino acids into MURG proteins using the general biosynthetic method of Noren, C. J., et al., Science, 244, pp. 182-188 (1989). In this method, the codon encoding the amino acid of interest in wild-type MURG is replaced by a "blank" nonsense codon, TAG, using oligonucleotide-directed mutagenesis (described in detail, infra). A suppressor tRNA directed against this codon is then chemically aminoacylated in vitro with the desired unnatural amino acid. The aminoacylated tRNA is then added to an in vitro translation system to yield a mutant MURG enzyme with the site-specific incorporated unnatural amino acid.

Selenocysteine or selenomethionine may be incorporated into wild-type or mutant MURG by expression of MURG-encoding cDNAs in auxotrophic E. coli strains. Hendrickson, W. A. et al., EMBO J., 9(5), pp. 1665-1672 (1990). In this method, the wild-type or mutagenized MURG CDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

The term "altered surface charge" means a change in one or more of the charge units of a mutant polypeptide, at physiological pH, as compared to wild-type MURG. This is preferably achieved by mutation of at least one amino acid of wild-type MURG to an amino acid comprising a side chain with a different charge at physiological pH than the original wild-type side chain.

The change in surface charge is determined by measuring the isoelectric point (pI) of the polypeptide molecule containing the substituted amino acid and comparing it to the isoelectric point of the wild-type MURG molecule.

The term "altered substrate specificity" refers to a change in the ability of a mutant MURG to cleave a substrate as compared to wild-type MURG.

The "kinetic form" of MURG refers to the condition of the enzyme in its free or unbound form or bound to a chemical entity at either its active site or accessory binding site.

A "competitive" inhibitor is one that inhibits MURG activity by binding to the same kinetic form, of MURG, as its substrate binds—thus directly competing with the

substrate for the active site of MURG. Competitive inhibition can be reversed completely by increasing the substrate concentration.

An "uncompetitive" inhibitor is one that inhibits MURG by binding to a different kinetic form of the enzyme than does the substrate. Such inhibitors bind to MURG already bound with the substrate and not to the free enzyme. Uncompetitive inhibition cannot be reversed completely by increasing the substrate concentration.

A "non-competitive" inhibitor is one that can bind to either the free or substrate bound form of MURG.

Those of skill in the art may identify inhibitors as competitive, uncompetitive or non-competitive, by computer fitting enzyme kinetic data using standard equations according to Segel, I. H., Enzyme Kinetics, J. Wiley & Sons, (1975). It should also be understood that uncompetitive or non-competitive inhibitors according to this invention may bind to the accessory binding site.

The term "homolog" means a protein having at least 25% amino acid sequence identity with MURG or any functional part of MURG, and including certain invariant amino acid residues corresponding to G14, G15, G18, H19, G104, H124, E125, G190, G191, S192, G194, A195, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E.coli* MurG sequence set forth in Figure 3a) and also including three glycine rich loops. A homolog may contain some or all of the invariant residues.

The term "co-complex" means MURG or a mutant or homologue of MURG in covalent or non-covalent association with a chemical entity or compound.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a MurG molecule or portions thereof. The association may be non-covalent--wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions--or it may be covalent.

The term ".beta.-sheet" refers to the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

The terms "atomic coordinates" or "structure coordinates" refer to mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a

MurG molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

The term "heavy atom derivatization" refers to the method of producing a chemically modified form of a crystal of MURG. In practice, a MurG crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thimerosal, uranyl acetate or mercuric chloride, which can diffuse through the crystal and bind to the surface of the protein. The location(s) of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the soaked crystal. This information, in turn, is used to generate the phase information used to construct three-dimensional structure of the enzyme. Blundel, T. L. and N. L. Johnson, Protein Crystallography, Academic Press (1976).

Those of skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the purpose of this invention, any set of structure coordinates for MURG or MURG homologues or MURG mutants that have a root mean square deviation of protein backbone atoms (N, C.alpha., C and O) of less than 0.75 Å when superimposed--using backbone atoms--on the structure coordinates listed in Table 1, Table 2 or Table 3 shall be considered identical.

The term "unit cell" refers to a basic parallelepiped shaped block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

The term "space group" refers to the arrangement of symmetry elements of a crystal.

The term "molecular replacement" refers to a method that involves generating a preliminary model of a MurG crystal whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known (e.g., MURG coordinates from Table 1, 2, or 3) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final,

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accurate structure of the unknown crystal. Lattman, E., "Use of the Rotation and Translation Functions", in Methods in Enzymology, 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York, (1972). Using the structure coordinates of MURG provided by this invention, molecular replacement may be used to determine the structure coordinates of a crystalline mutant or homologue of MURG or of a different crystal form of MURG.

DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to the discovery of the three-dimensional structure of the crystalline form of the *E. coli* MurG protein, models of such three-dimensional structures, a method of structure based drug design using such structures, methods to identify ligands or compounds that interact or bind with such structures, the compounds identified by such methods, and the use of such compounds in therapeutic compositions.

More particularly, the present invention relates to novel crystals of *E. coli* MurG protein, methods of production of such crystals, three dimensional coordinates of MurG protein, MurG structures and models derived from the *E. coli* MurG structure, and uses of such structures and models to derive other MurG structures and in ligand discovery and drug design strategies.

The present invention also relates to three-dimensional structures and coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, structures and models of the binding sites, and uses of such structures and models to derive the binding sites of other MurG proteins and in drug design strategies.

Solely for ease of explanation, the description of the invention is divided into the following sections: (1) crystals of MurG protein; (2) methods of crystallization; (3) three-dimensional crystal coordinates and structure of *E. coli* MurG; (4) three-dimensional coordinates and structure of the donor nucleotide binding site of MurG; (5) coordinates and structure of the acceptor binding site of MurG; (5) three dimensional coordinates and structure of the membrane association site; (6) two dimensional and three dimensional images of the protein, α-carbon backbone, α-carbon backbone with conserved amino

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acid residues, and binding sites; and (7) computer readable mediums comprising the three dimensional coordinates of the MurG protein, α-carbon backbone, α-carbon backbone with conserved amino acid residues, and binding sites; (8) images of structures of MurG protiensand binding sites; (9) models of MurG proteins and binding sites thereof and methods of using the structure of MurG to determine the structures of other MurG proteins and binding sites; (10) structure based drug design using models of MurG protein and binding site structures; (11) compounds derived from structure based drug design; and (12) therapeutic compositions using drugs designed from structure based drug design.

CRYSTALS

One embodiment of the present invention includes a composition comprising a MurG protein in a crystalline form (i.e., MurG crystals). As used herein, the terms (crystalline MurG" and "MurG crystal" both refer to crystallized MurG protein and are intended to be used interchangeably. More particularly, an embodiment of the present invention includes a composition comprising an *E. coli* MurG protein in a crystalline form. Preferably, a crystalline MurG is produced using the crystal formation method described herein, in particular according to the method disclosed in Example 1. A MurG crystal of the present invention comprises any crystal structure and preferably precipitates as a triclinic crystal. Preferably, a composition of the present invention includes MurG crystal molecules arranged in a crystalline manner in a P1 space group with two molecules per assymmetric unit so as to form a unit cell of dimensions a=60.613 Å, b=66.356 Å, c=67.902 Å, α=64.294, β=83.520, γ=65.448. A preferred crystal of the present invention provides X-ray diffraction data for determination of atomic coordinates to a resolution of about 3.0 Å, preferably to about 2.4 Å, and more preferably to about 1.8 Å.

Another embodiment of the present invention includes crystalline MurG protein co-crystallized with a donor nucleotide or substrate or substrate analog. Preferably, a donor nucleotide is UDP or UDP-GlcNAc (UDP-N-acetylglucosamine) or an analog thereof. The substrate or substrate analog is preferably Lipid I or Lipid II, or analogs of Lipid I or Lipid II. More specifically, Lipid I and II analogs are as described in PCT/US99/02187, published as WO99/38958 and US Provisional Application Nos.

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60/122,966 filed March 3, 1999 and 60/137,696 filed June 4, 1999, and International Application No. PCT/US00/05554 entitled "Bacterial transglycosylases: Assays for monitoring the activity using lipid II substrate analogs and methods for discovering antibiotics," all incorporated herein by reference in their entirety.

Included in the present invention, a variety of MurG proteins from numerous organisms can be used to prepare MurG crystals, including but not limited to, microorganisms such as bacteria, higher-order bacteria, thermal stable bacteria, spirochetes, small pathogenic organisms, fungi, protozoa, cyanobacteria, and trypanosomes. More particularly, bacteria such as but not limited to, *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii,Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.*

In another embodiment of the present invention, the MurG proteins or fragments thereof, mutants or homologs are expressed in, for example, an *E. coli* host cell for use expressing sufficient quantities of sufficiently purified protein to form crystals. The present inventors have demonstrated that it is possible to express *Enterococcus. faecalis* MurG in *E. coli* cells — so the MurG proteins from many organisms can be cloned into expression vectors suitable for expression in *E. coli* cells. This would facilitate obtaining sufficient quanitites of isolated or purified MurG proteins. The expression of *E. faecalis* MurG protein in *E. coli* host cells is performed, for example, by expressing the *E. faecalis* MurG gene cloned into a pET21b expression vector and transformed into an *E. coli* host cell. The MurG protein is over-expressed with a C-terminal his tag (LEHHHHHH) which allows the protein to be purified using a His-tag affinity column. The protein is then crystallized and the atomic coordinates are determined using X-ray diffraction and methods known to those skilled in the art.

It is another embodiment of the present invention to provide for the construction and expression of chimeric MurG proteins to enable the crystallization and determination of the three dimensional coordinates of such chimeras. For example, if there are problems obtaining or crystallizing MurGs from other organisms, the present invention

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provides information that makes it possible to make chimaeric proteins containing the donor or acceptor binding site from *E. coli* MurG and the corresponding acceptor or donor binding site from another organism. Chimaeric proteins could be easier to express, handle, or crystallize. For example, we have found that E. faecalis MurG is more difficult to solubilize that *E. coli* MurG (requiring more detergent). It is believed that the problems are related to the acceptor binding domain having a stronger affinity for the bacterial membranes. To overcome this problem, one can attach the donor binding domain of *E. faecalis* to the *E. coli* acceptor binding site and determine structure to see details of *E. faecalis* donor binding domain.

According to the present invention, crystalline MurG can be used to determine the ability of a chemical compound to bind to a MurG protein in a manner predicted by a structure based drug design method of the present invention. Preferably, a MurG crystal is soaked in a solution containing a chemical compound of the present invention. Binding of the chemical compound to the crystal is then determined by methods standard in the art. Thereby, the co-crystal of MurG and a compound of interest is determined.

METHODS OF CRYSTALLIZATION

The present invention includes a method for producing crystals of MurG proteins, comprising: combining MurG protein with a reservoir solution and inducing crystal formation to produce MurG crystals. Another embodiment of the present invention, a method for producing crystals of MurG protein comprises combining MurG protein with UDP-GlcNAc in a 1:3 ratio and with a reservoir solution and inducing crystal formation to produce MurG crystals.

Preferably, crystals of MurG are formed using a solution containing a range of MurG protein from about 1 mg/ml to about 20 mg/ml, more preferably above 5 mg/ml, limited only by the solubility of the protein, which may vary depending on the specific amino acid sequence.

A reservoir solution contains the buffer, the precipitant, and additives if necessary. A suitable reservoir buffer of the present invention comprises NaMES (2-[N-morpholino]ethanesulfonic acid, sodium salt) buffer, NaHEPES (N-[2-hydroxyethyl]piperazine-N'-[2-ethanesulfonic acid, sodium salt) buffer, Tris (tris[hydroxymethyl]aminomethane) buffer, and any buffer which has the PKa between

5.5 and 8.0. A suitable NaMES buffer solution has a pH range from about 5.6-6.5. Most preferably, the NaMES buffer has a pH of about 6.5. The precipitant comprises ammonium sulfate, saturated sodium and potassium tartrate and polyethylene glycol. A suitable concentration of ammonium sulfate can range from 0.8 M to 1.5 M. Most preferably, the ammonium sulfate concentration is about 0.96 M. A suitable additive comprises detergents like Triton X-100 and n-octyl-beta-glucoside. The concentration of Triton X-100 can range from 0.1% to 1%. Most preferably, the concentration of Triton X-100 is 0.4%.

In a preferred embodiment, MurG crystals are produced by a method comprising concentrating MurG protein in a buffer solution, mixing the protein concentrate with UDP-GlcNAc in a 1:3 molar ratio, mixing equal volumes of protein solution with a reservoir solution, and inducing crystal formation to produce MurG crystals.

In a particular embodiment of the invention, MurG crystals are produced by a method comprising concentrating MurG protein to 10 mg/ml in a buffer of 20 mM Tris-HCl, pH 7.9/150mM NaCl and 50 mM EDTA; mixing the protein concentrate with UDP-GlcNAc in a 1:3 molar ratio; mixing equal volumes of protein solution with a reservoir solution comprising (0.1 M NaMES, pH 6.5, 0.96 M $(NH_4)_2SO_4$, 0.4% TRITON® X-100, and 10 mM dithiolthreitol (DTT)), and inducing crystal formation using hanging drop vapor-diffusion.. This preferred method is described in greater detail in Example 1.

Supersaturated solutions of MurG protein can be induced to crystallize by several methods including, but not limited to, vapor diffusion, liquid diffusion, batch crystallization, constant temperature and temperature induction or a combination thereof. Preferably, supersaturated solutions of MurG protein are induced to crystallize by vapor diffusion (i.e., hanging drop method). In a vapor diffusion method, a MurG protein solution is combined with a reservoir solution of the present invention that will cause the MurG protein solution to become supersaturated and form MurG crystals at a constant temperature. Vapor diffusion is preferably performed under a controlled temperature in the range of from about 15°C to about 30°C, more preferably from about 20°C to about 25°C, and most preferably at a constant temperature of about 22°C.

In another preferred embodiment, the present invention includes a method to produce crystals of MurG protein comprising the steps of: (a) preparing an about 10

mg/ml solution of MurG protein in a Tris-HCl buffer, (b) mixing UDP-GlcNAc with the MurG protein solution in a 3:1 molar ratio, (c) dropping 2 μl droplet of this protein sample onto a coverslip, (d) adding an equal volume of reservoir solution to this droplet and inverting this over a well containing about 1 ml of the reservoir solution; and (e) incubating until crystals of MurG form.

Any isolated MurG protein can be used with the present method. An isolated MurG protein can be isolated from its natural milieu or produced using recombinant DNA technology (e.g., polymerase chain reaction (PCR) amplification, cloning) or chemical synthesis. To produce recombinant MurG protein, a nucleic acid molecule encoding a MurG protein can be inserted into any vector capable of expressing the nucleic acid in a host cell. Suitable and preferred nucleic acid molecules to include in recombinant vectors of the present invention are as disclosed herein. Such suitable and preferred nucleic acid molecules include numerous MurG encoding genes that have been isolated to date, and that will be isolated in the future. A preferred nucleic acid molecule of the present invention encodes a homologue of MurG. Homologues of MurG can be recognized by the presence of certain conserved amino acid residues or sequences.

A sequence alignment for six MurG sequences is shown in fig. 3A. Highlighted residues include those that are invariant or almost invariant across all MurG proteins. A nucleic acid molecule of the present invention can encode any portion of a MurG protein, preferably a full-length MurG protein or either of the two domains. A more preferred nucleic acid molecule to include in a recombinant vector, and particularly in a recombinant molecule, includes a nucleic acid molecule encoding a protein having the amino acid sequence represented by amino acid sequences of MurG proteins as deposited in the NCBI database and are identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552,)67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640,

AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436. Further, examples of nucleic acid molecules encoding MurG proteins have been deposited in NCBI, Genbank, and have Accession Nos. AL162758, AE002281, D90917, AF110367, AL139077, AJ242646, AE000520, AE000511, L42023, U00096, NC-000922, AE000783, AE000657, AE001348, AF099188, AR048673, AR048672, AF179611, AL022602, AL109663, X55034, AE000621, D10602, AE001670, X64259, Y13922, U10879, AE001535, AF068902, AJ235271, AE000118, AE001227, AE001176, U94707, Z95388, U32793, AE000727, D84504, Z99111, D10483,X52644, X52540, and L24773. These sequences are known and are publicly available. Further, as additional genomes and genes are sequenced, more MurG encoding nucleotide sequences will become available, and can be used in the present invention.

In specific embodiments of the invention, the protein sequence of *E. coli* MurG was reported in 1990 (Ikeda et al. Nucleic Acids Res. 1990, 19:4014; and Mengin-Lecreuix, D. et al., Nucleic Acids Res. 1990, 18:2810.). *E. coli* genomic DNA can be purified from *E. coli* or purchased from ATCC, or the gene for *E. coli* MurG is cloned into a plasmid can be obtained from numerous sources. Primers were designed to the portions of the gene corresponding to the N and C termini of the protein. The primers also encoded restriction enzyme sites outside the protein coding region. The gene sequence was amplified; the corresponding double stranded nucleic acid molecule was cut with appropriate restriction enzymes for cloning into a commercially available expression vector (pET expression vectors available from Novagen provide for numerous variations of MurG protein – wild-type or fusion proteins or proteins with affinity tags at N or C terminus. We have worked with several constructs but found that MurG with a His-tag at C-terminus crystallized best; the protein sequence contained an extra methionine at N-terminus and eight extra residues at C terminus, six of which were histidines. The vector used was pET21b. (as described in Ha et al. J. Am. Chem. Soc. 121, (1999) 8415-8426 hereby incorporated by reference in its entirety).

A recombinant vector of the present invention can be either RNA (probably not) or DNA, and typically includes, but is not limited to, a virus or plasmid. Any recombinant vector and host cell that provides for expression of a MurG protein

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encoding mucleic acid sequence can be used in the present invention to express MurG protein for crystallization. Preferred vectors are engineered for high level expression in E. coli such as, but not limited to, pET vectors. We have found that over-expression of Murg from either *E. coli* or *E. faecalis* in *E. coli* cells is not toxic and, thus, this approach will work for other MurG proteins.

As used herein, an expression vector is a DNA vector that is capable of transforming a host cell and of affecting expression of a specified nucleic acid molecule. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including bacterial, fungal, and other microorganisms cells. Preferred expression vectors of the present invention direct expression in bacterial cells from a plasmid. A preferred recombinant molecule of the present invention comprises pET21b with E. coli MurG gene cloned into the Nde1 and Xho1 sites.

An expression vector of the present invention can be transformed into any suitable host cell to form a recombinant cell. A suitable host cell includes any cell capable of expressing a nucleic acid molecule inserted into the expression vector. For example, a procaryotic expression vector can be transformed into a bacterial host cell. If the expression vector contains a T7 promoter then a source of T7 RNA polymerase must be provided to induce expression. Some host cells contain the T7 RNA polymerase gene in a repressed state. Expression of T7 RNA polymerase can be induced with a chemical signal such as IPTG or heat. Alternatively, a source of T7 RNA polymerase can be introduced at the appropriate time by infection with a phage containing a copy of T7 RNA polymerase. A wide range of hosts strains can be infected with a suitable phage. Some host strains have been engineered to contain inducible copies of T7 RNA polymerase gene. Such host strains include BL21(DE3) and derivatives thereof. A preferred host strain of the present invention is BL21(DE3)pLysS or BL21(DE3)pLysE, which are commercially available from Novagen and can be readily transformed with a DNA plasmid vector containing a MurG gene under the control of the T7 promoter. As already stated above, a preferred vector is a pET vector, preferably containing a restriction enzyme site permitting cloning of the gene as a fusion containing a C-terminal his tag.

In a preferred embodiment, one method to isolate MurG protein useful for producing MurG crystals includes recovery of MurG protein having a C-terminal LEHHHHHH (His tag) sequence purified as described in Ha *et al.* (1999, J. Amer. Chem. Soc. 121:8415-8426). One of skill in the art is able to modify this procedure in order to purify other proteins can be produced as C-terminal histadine (his) tags. The purification conditions for specific MurG proteins will vary depending upon the particular characteristics of the proteins such as their isoelectric point, molecular weight, etc. It is known that the isoelectric points of different Murg homologues vary a bit, although they are generally relatively high. Also, some Murg homologues may be more hydrophobic than others, which will mean differences in amount of detergent necessary for purification. It is likely that all the Murg homologues can be purified over nickel affinity columns using the C-terminal his-tag as a handle. Those skilled in the art of protein purification will know how to modify purification parameters depending upon the protein characteristics, in order to purify the protein for crystallization.

STRUCTURE OF MURG PROTEIN

One embodiment of the present invention includes a model of a MurG protein, in which the model represents a three dimensional structure of a MurG protein. Another embodiment of the present invention includes the three dimensional structure of a MurG protein. A three dimensional structure of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 1. According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 1) to allow the three dimensional structure of another MurG protein to be modeled or calculated using the particular set of atomic coordinates defining the three dimensional configuration of the MurG protein. For example, but not meant to be a limitation, homology modeling can be done using the linear sequence of a different MurG and E. coli coordinates; molecular replacement can allow the solution of a different MurG structure using the *E. coli* MurG coordinates and experimental data such as x-ray diffraction pattern from a different MurG crystal. According to the present invention, a three dimensional structure of a

given portion or chain of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the α-carbon or C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of amino acid side chains. As used herein, the phrase "common amino acid side chains" refers to amino acid side chains that are common to both the structure which substantially conforms to a given set of atomic coordinates and the structure that is actually represented by such atomic coordinates. Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the common amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å.

In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the common amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the common amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the common amino acid side chains have the recited average RMSD value.

In more preferred embodiments of the present invention, a large number of different "rotamers" or "rotational isomers" of the MurG protein are encompassed by three dimensional structures of the invention in which the amino acid side chains are at a variety of positions in crystalline forms of the protein or for the protein in solution. Different rotamers refer to molecules of identical configuration may be distinguished as having different conformations after rotation about the various molecular bonds. Therefore, while the same or similar amino acids may be present, the exact location will vary depending upon the freedom of rotation of the bonds due to hydrogen bonding, and other molecular forces.

STRUCTURE OF THE α-CARBON BACKBONE OF MURG AND THE α-CARBON BACKBONE AND CONSERVED AMINO ACID RESIDUES

The present invention includes the three dimensional structure of the α-carbon or C-alpha backbone of a MurG protein, in particular the *E. coli* MurG protein. A three dimensional structure of the C-alpha backbone of the MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 2.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value. The C-alpha backbone of MurG proteins is expected to be more conserved than the location of the particular amino acid residue side chains.

The present invention also includes the three dimensional structure of the α-carbon or C-alpha backbone and conserved or invariant amino acid residue side chains of a MurG protein, in particular the E. coli MurG protein. A three dimensional structure of the C-alpha backbone and conserved amino acid residues of the MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 3. The conserved amino acids are highlighted in blue in Figure 3a and include G14, G15, G18, H19, G104, H124, E125, G190, G191, S192, G194, A195, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the E. coli MurG sequence set forth in Figure 3a).

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the C-alpha backbone and conserved amino acid residue atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

STRUCTURE OF THE DONOR NUCLEOTIDE BINDING SITE OF MURG PROTEINS

An embodiment of the present invention includes the three dimensional structure of a donor nucleotide binding site of a MurG protein, in particular an E. coli MurG protein. A more preferred embodiment of the present invention includes a three dimensional structure of a donor nucleotide binding site of a MurG protein wherein the three dimensional structure of the donor nucleotide binding site substantially conforms to the atomic coordinates in Table 4. In a preferred embodiment, the donor nucleotide binding site is a UDP-GlcNAc binding site of a MurG protein.

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As described in Example 1, the donor nucleotide binding site is located in the C-terminal domain (see Fig. 4a). This binding site is based on the comparison of β-glucosyltransferase (BGT) and *E. coli* MurG and based on experiments done in our laboratory showing that the isolated C domain binds to a UDP-hexose column (See Example 1). The atomic coordinates of Table 4 set forth the donor nucleotide binding site three dimensional structure without a donor nucleotide such as UDP-GlcNAc bound to the MurG protein.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of a donor nucleotide binding site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 4) to allow the three dimensional structure of the donor nucleotide binding domain to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates defining the three dimensional configuration of the donor nucleotide binding site of a MurG protein. According to the present invention, a three dimensional structure of a given donor nucleotide binding site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG. Since the atomic coordinates of Table 4 were obtained from the *E. coli* MurG crystal protein without a donor nucleotide bound, there will be some variation from the atomic coordinates of the donor nucleotide binding site when a nucleotide is bound vs. unbound. Therefore, a structure "substantially conforming" to that represented by the atomic coordinates in Table 4, will include a structure obtained from co-crytallization of the protein with a donor nucleotide.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 1.3 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and more preferably less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that

substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of the conserved or invariant amino acid side chains located within the binding site. As used herein, the phrase "conserved amino acid side chains" refers to amino acid side chains that are conserved between MurG proteins within the donor nucleotide binding site. The conserved amino acid residues of the donor nucleotide binding site have been identified as I125, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a) and the G loop found between residues numbered 190-195 having residues G190, G191, S192, G194, and A195. Some or all of these conserved residues are necessary for binding the nucleotide donor.

Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the conserved amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the conserved amino acid side chains have the recited average RMSD value.

STRUCTURE OF THE ACCEPTOR BINDING SITE OF MURG PROTEIN

An embodiment of the present invention includes the three dimensional structure of an acceptor binding site of a MurG protein. A three dimensional structure of a acceptor binding site of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 5. A more preferred embodiment of the present invention includes a three dimensional structure of an

acceptor binding site of a MurG protein wherein the three dimensional structure of the acceptor binding site substantially conforms to the atomic coordinates Table 5.

According to the present invention, the use of the term "acceptors" refers to Lipid I and analogues thereof. For the purposes of obtaining co-crystals containing acceptor analogues bound to the acceptor binding site better, the analogues need not be functional acceptors in a MurG assay. In particular embodiments of the present invention, the acceptor is selected from the group consisting of, but not limited to Lipid I, and analogs of Lipid I (see compounds described in Ha et al., J. Amer. Chem. Soc. 1999, vol. 121:8415-26, incorporated by herein by reference in its entirety).

As described in Example 1, the acceptor binding site is located in the N-terminal domain of a MurG protein (see Fig. 3a and 4c). The acceptor binding site or domain is characterized by three highly conserved regions, two of which are glycine-rich loops (also referred to as "G loops") that face the cleft between the C-terminal and N-terminal domains. The conserved residues of the acceptor binding site comprise G14, G15, G18, H19, G104, H124, and E125 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a) and two conserved G loop structures.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of an acceptor binding site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 5) to allow the three dimensional structure of the acceptor binding site to be modeled or calculated (i.e., by homology modeling) using the particular set of atomic coordinates defining the three dimensional configuration of the acceptor binding site of a MurG protein. According to the present invention, a three dimensional structure of a given acceptor binding site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of the conserved amino acid side chains. As used herein, the phrase "conserved amino acid side chains" refers to the conserved or invariant amino acid side chains that are common to MurG proteins. Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a

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structure wherein at least about 50% of the conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the conserved amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the conserved amino acid side chains have the recited average RMSD value.

STRUCTURE OF A MEMBRANE ASSOCIATION SITE OF MurG PROTEIN

An embodiment of the present invention includes the three dimensional structure of a membrane association site of a MurG protein. A three dimensional structure of a membrane association site of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 6. A more preferred embodiment of the present invention includes a three dimensional structure of an acceptor binding site of a MurG protein wherein the three dimensional structure of the acceptor binding site substantially conforms to the atomic coordinates in Table 6.

According to the present invention, the use of the term "membrane association site" refers to the region of a MurG protein that associates with cytoplasmic surface of bacterial membranes where it performs the reaction of coupling a soluble donor sugar to the membrane anchored acceptor sugar, Lipid I. Analysis of the *E. coli* MurG protein structure shows a hydrophobic patch consisting of residues I75, L79, F82, W85, and W116 in the N-domain. The membrane association site is where the MurG protein associates with the bacterial membranes, and that it is target for inhibitors if we find that a) we can bind to it with another molecule; b) we can disrupt membrane association by binding to it; or c) disrupting membrane association inhibits activity.

As described in Example 1, the membrane association site is located in the N-terminal domain of a MurG protein (see Fig. 4c). The location of the membrane association site is in close proximity to the acceptor binding site and membrane

association in this patch would bring the two M-terminal G-loops close to the membrane surface where the diphosphate portion of the acceptor is located.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three dimensional structure of a membrane association site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 6) to allow the three dimensional structure of the membrane association site to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates defining the three dimensional configuration of the membrane association site of a MurG protein. According to the present invention, a three dimensional structure of a given membrane association site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three dimensional configuration of a second MurG.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the structural elements in the site, and more preferably, less than about 1.3 Å for the structure elements in each site, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and more preferably, less than about 0.3 Å for the structural elements in each site. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of α-carbon backbone and conserved amino acid side chains. As used herein, the phrase "conserved amino acid side chains" refers to amino acid side chains that are conserved between MurG proteins. Preferably, a three dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved α-carbon backbone and conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less

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than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the α-carbon backbone and conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the α-carbon backbone and conserved acid side chains have the recited average RMSD value, and most preferably, about 100% of the α-carbon and conserved amino acid side chains have the recited average RMSD value.

COMPUTER READABLE MEDIUM

Another embodiment of the present invention relates to a computer-readable medium encoded with, a set three dimensional coordinates seleceted from the group consisting of the three dimensional coordinates represented in Table1, the three dimensional coordinates represented in Table 2, the three dimensional coordinates represented in Table 3, the three dimensional coordinates represented in Table 4, the three dimensional coordinates represented in Table 5, or the three dimensional coordinates represented in Table 6, wherein using a graphical display software program, the three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image. Preferably, the three dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

Yet another embodiment of the present invention relates to a computer-readable medium encoded with a set of three dimensional coordinates of a three dimensional structure which substantially conforms to the three dimensional coordinates represented in Table 1, wherein using a graphical display software program, the three dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image. In other embodiments, the present invention relates to a computer-readable medium encoded with a set of three dimensional coordinates of a three dimensional structure which substantially conforms to the three dimensional coordinates represented in Table 2, Table 3, Table 4, Table 5 or Table 6, wherein using a graphical display software program, the three dimensional

coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three dimensional image. Preferably, the three dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

IMAGES

One embodiment of the present invention relates to a two dimensional image of an *E. coli* MurG protein including those illustrated in Figures 3-4. Most of these figures were drawn with the MOLSCRIPT program. Preferably, the two dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

Another embodiment of the present invention includes a three dimensional computer image of the three dimensional structure of a MurG protein, preferably the *E. coli* MurG protein. Suitable structures of which to produce three dimensional computer images are disclosed herein. Preferably, a computer image is created to a structure substantially conforming with the three dimensional coordinates represented in Table 1.

Another embodiment of the present invention includes an image of an MurG protein that is generated when a set of three dimensional coordinates comprising the three dimensional coordinates represented in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file as a three dimensional image. Suitable structures to image are disclosed herein. Preferably, the three dimensional structures are of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG. Most preferably, the MurG protein is the *E. coli* MurG protein described herein. A computer image of the present invention can be produced using any suitable software program, including, but not limited to, MOLSCRIPT 2.0 (Avatar Software AB, Helenebrgsgatan 21C, SE-11713, Stockholm, Sweden), the graphical display program O (Jones et al., Acta

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Crystallography, vol. A47, p. 110, 1991), or the graphical display program GRASP. Suitable computer hardware useful for producing an image of the present invention are known to those of skill in the art. Preferred computer hardware includes a Silicon Graphics Workstation.

MODELS OF MURG PROTEINS AND BINDING SITES

According to the present invention, a three dimensional structure of the *E. coli* MurG protein and its binding sites of the present invention can be used to derive a model of the three dimensional structure of another MurG protein and its binding sites (i.e., a structure to be modeled). As used herein, a "structure" of a protein refers to the components and the manner of arrangement of the components to constitute a protein or binding site. Also, as used herein, the term "model" refers to a representation of a tangible medium of the three dimensional structure of a protein, polypeptide or peptide, or binding site of a protein. For example, a model can be a representation of the three dimensional structure in a electronic file, on a computer screen, on a piece of paper (i.e., on a two dimensional medium), and/or as a ball-and-stick figure. Physical three-dimensional models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, and Biosym Technologies, San Diego, CA. The phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Computer screen images and pictures of the model can be visualized in a number of formats including space-filling representations, α carbon traces, ribbon diagrams and electron density maps.

Suitable target MurG proteins and their associated binding sites to model using a method of the present invention include any MurG protein and binding sites that are at least in part structurally related to the *E. coli* MurG protein or its binding sites. A preferred target MurG structure that is at least in part structurally related includes a target MurG structure having an amino acid sequence that is at least about 25%, preferably at least about 30%, more preferably at least about 36%, more preferably at least about 40%,

even more preferablye at least about 50%, more preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80%, and more preferably at least about 90% identical to an amino acid sequence of the *E. coli* MurG protein, across the full-length of the target MurG structure sequence when using, for example, a sequence alignment program such as DNAsis™ program (available from Hitachi Software, San Bruno, CA) or the MacVector™ program (available from the Eastman Kodak Company, New Haven, CT) or the GCγ™ program (available from the "GCγ", University of Wisconsin, Madison, WI), such alignment being performed for example, using the standard default values accompanying such alignment programs.

Preferred MurG proteins and their binding sites are set forth in the amino acid sequences of MurG proteins as deposited in the NCBI database and are identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436. The amino acid sequences are publicly available.

A variety of MurG proteins from numerous organisms can be used to prepare models of MurG proteins and binding sites, including but not limited to, microorganisms such as bacteria, higher-order bacteria, thermal stable bacteria, spirochetes, small pathogenic organisms, fungi, protozoa, cyanobacteria, and trypanosomes. More particularly, bacteria such as but not limited to, *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coelicolor, Streptomyces collinus, Streptococcus*

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pneumoniae, Synechocystis sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.* It is noted that nucleotide and amino acid sequences for many of the above identified organisms are known and publicly available.

Preferred target MurG proteins and binding site structures to model also include, but are not limited to, derivatives of MurG proteins, such as a MurG protein having one or more amino acid residues substituted, deleted or added (referred to herein as MurG mutants), or proteins encoded by natural variants of a nucleic acid molecule encoding a MurG.

In another embodiment of the invention, the process of building a homology model for a protein is divided into the following steps:

(1) Determine which proteins are related to the model protein;

(2) Determine structurally conserved regions (SCRs);

(3) Align the amino acid sequence of the unknown protein with those of the reference protein(s) within the SCRs;

(4) Assign coordinates in the conserved regions;

(5) Predict conformations for the rest of the peptide chain, including loops between the SCRs and possibly the N- and C-termini;

(6) Search for the optimum side chain conformations for residues that differ from those in the reference proteins; and

(7) Use energy minimization and molecular dynamics to refine the molecular structure so that steric strain introduced during the model-building process can be relieved.

Published sequences are readily available through on-line databases on the Internet, such as SwissProt (http://www.expasy.ch/sprot/sprot-top.html). MurG specific and related sequences are obtained for use for building homology models by text-based or sequence similarity searching. SCRs for MurG is the entire protein, considering the E. coli MurG crystal structure is the only similar sequence with structural data. Alignment of the sequences using an appropriate alignment program and algorithm, such as Clustal W, allows appropriate assignment of the E. coli protein coordinates to a MurG sequence of unknown structure. The Modeler program performs the conformational predictions

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for the peptide chain and side chains. Dynamics and minimization using an appropriate program and algorithm, such as Discover.

Modeler Description:

Modeler is an automated homology-modeling scheme designed to find the most probable three-dimensional structure of a protein, given its amino acid sequence and its alignment with related structures. It derives 3D protein models without the time consuming separate stages of core region identification and loop region building or searching that is inherent to manual homology modeling schemes. The related or reference protein structures are used to derive spatial restraints expressed as probability density functions (PDFs) for each of the restrained features of the model. As an example, the main chain conformation of a given residue in the model will be described by restraints that depend upon the residue type, the main chain conformation of equivalent residues in the reference proteins and the local sequence similarity. The probability distribution functions that are used in restraining the model structure are derived from correlations between structural features in a database of families of homologous proteins aligned on the basis of their 3D structure. These functions are used to restrain C-C distances, main chain N--O distances, main chain and side chain dihedral angles, etc. The individual restraints are assembled into a single molecular probability density function (MPDF). The three-dimensional protein model is then obtained by an optimization of this MPDF. The optimization procedure itself consists of a variable target function method (Braun and Go, 1985) with conjugate gradient minimization scheme followed by an optional restrained simulated annealing molecular dynamics scheme.
While several reference structures are used in the traditional homology model building process, only one set of coordinates can be used in any one peptide segment. Modeler is able to simultaneously incorporate structural data from one or more reference proteins. Structural features in the reference proteins are used to derive spatial restraints which in turn are used to generate model protein structures using conjugate gradient and simulated annealing optimization procedures.

Clustal W description:

Clustal W aligns multiple sequences using a progressive pairwise alignment algorithm. It first generates all possible pairwise alignments for a list of sequences and then builds the guide tree based on their pairwise sequence identity, aligning the sequences following the order of the guide tree.

Several unique features in Clustal W improve the sensitivity of the alignment of divergent protein sequences (Thompson et al, 1994a).

(1) Individual weights are assigned to each sequence in a partial alignment in order to downweight near-duplicate sequences and upweight the most divergent ones.

(2) Amino acid substitution matrices are varied at different alignment stages according to the divergence of the sequences to be aligned.

(3) Residue-specific gap penalties and locally reduced gap penalties in hydrophilic regions encourage new gaps in potential loop regions rather than regular secondary structure.

(4) Positions in early alignments, where gaps have been opened, receive locally reduced gap penalties to encourage the opening of new gaps at these positions.

Discover Description:

The Discover program performs energy minimization, template forcing, torsion forcing, and dynamic trajectories and calculates properties such as interaction energies, derivatives, mean square displacements, and vibrational frequencies. It provides tools for performing simulations under various conditions including constant temperature, constant pressure, constant stress, periodic boundaries, and fixed and restrained atoms.

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STRUCTURE BASED DRUG DESIGN

The present invention relates to the use of the crystal structure of the *E. coli* MurG protein represented by the atomic coordinates in Table 1 to make models of MurG proteins and binding sites thereof. The present invention also relates to the use of the crystal structure, α-carbon backbone, α-carbon backbone plus conserved amino acid residue side chains or binding sites of the *E. coli* MurG protein to construct models of these structures in other MurG proteins.

For the first time, the present invention permits the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site or accessory binding site of MURG, in whole or in part.

On approach enabled by this invention, is to use the structure coordinates of MURG to design compounds that bind to the enzyme and alter the physical properties of

the compounds in different ways, e.g., solubility. For example, this invention enables the design of compounds that act as inhibitors of the MURG enzyme by binding to, all or a portion of, the active site of MURG.

A second design approach is to probe a MurG crystal with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate MURG inhibitors and the enzyme. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each tpe of solvent molecule sticks. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their MURG inhibitor activity. Travis, J., Science, 262, p. 1374 (1993).

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to MURG, with MURG. Thus, the time-dependent analysis of structural changes in MURG during its interaction with other molecules is enabled. The reaction intermediates of MURG can also be deduced from the reaction product in co-complex with MURG. Such information is useful to design improved analogues of known MURG inhibitors or to design novel classes of inhibitors based on the reaction intermediates of the MURG enzyme and MURG-inhibitor co-complex. This provides a novel route for designing MURG inhibitors with both high specificity and stability.

Another approach made possible and enabled by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to the MURG enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. Meng, E. C. et al., J. Coma. Chem., 13, pp. 505-524 (1992).

Because MURG may crystallize in more than one crystal form, the structure coordinates of MURG, or portions thereof, as provided by this invention are particularly useful to solve the structure of those other crystal forms of MURG. They may also be used to solve the structure of MURG mutants, MURG co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of MURG.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of MURG, a MurG mutant, or a MurG co-complex, or the crystal of some other protein with significant amino acid sequence homology to any functional domain of MURG, may be determined using the MURG structure coordinates of this invention as provided in Tables 1-6. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information ab initio.

In addition, in accordance with this invention, MURG mutants may be crystallized in co-complex with known MURG inhibitors. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type MURG. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between MURG and a chemical entity or compound.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 2-3 .ANG. resolution X-ray date to an R value of about 0.20 or less using computer software, such as X-PLOR (Yale University, .COPYRGT.1992, distributed by Molecular Simulations, Inc.). See, e.g., Blundel & Johnson, supra; Methods in Enzvmoloav, vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985). This information may thus be used to design, synthezie and optimize novel classes of MURG inhibitors.

The structure coordinates of MURG mutants provided in this invention also facilitate the identification of related proteins or enzymes analogous to MURG in function, structure or both, thereby further leading to novel therapeutic modes for treating or preventing UDP-glycosyltransferase mediated diseases.

The design of compounds that bind to or inhibit MURG according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with MURG. Non-covalent molecular interactions important in the association of MURG with its substrate include hydrogen bonding, van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with MURG. Although certain portions of the compound will not directly

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participate in this association with MURG, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., active site or accessory binding site of MURG, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with MURG.

The potential inhibitory or binding effect of a chemical compound on MURG may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and MURG, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to MURG and inhibit using the assay of Walker et al. patents (cited supra). In this manner, synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of MURG may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of MURG.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with MURG and more particularly with the individual binding pockets of the MURG donor nucleotide binding site, acceptor binding site or membrane association site. This process may begin by visual inspection of, for example, the binding sites on the computer screen based on the MURG coordinates in Tables 1-6. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within an individual binding pocket of MURG as defined supra. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities, including but not limited to:

1. GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules" J. Med. Chem., 28, pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.

2. MCSS (Miranker, A. and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, Mass.

3. AUTODOCK (Goodsell, D. S. and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing" Proteins: Structure. Function, and Genetics, 8, pp. 195-202 (1990)) (AUTODOCK is available from Scripps Research Institute, La Jolla, Calif.).

4. DOCK (Kuntz, I. D. et al., "A Geometric Approach to Macromolecule-Ligand Interactions" J. Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, Calif.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may be proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of MURG. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include, but are not limited to:

1. CAVEAT (Bartlett, P. A. et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules". In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989)). CAVEAT is available from the University of California, Berkeley, Calif.

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif.). This area is reviewed in Martin, Y. C., "3D Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992)).

3. HOOK (available from Molecular Simulations, Burlington, Mass.).

Instead of proceeding to build a MurG inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other MURG binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include, but are not limited to:

1. LUDI (Bohm, H.-J., "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. ComR. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, Calif.

2. LEGEND (Nishibata, Y. and A. Itai, Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, Mass.

3. LeapFrog (available from Tripos Associates, St. Louis, Mo.).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., Cohen, N. C. et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, Navia, M. A. and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to MURG may be tested and optimized by computational evaluation. For example, a compound that has been designed or selected to function as a MurG-inhibitor must also preferably traverse a volume not overlapping that occupied by the active site when it is bound to the native substrate. An effective MURG inhibitor must preferably demonstrate a relatively small difference in

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energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient MURG inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, preferably, not greater than 7 kcal/mole. MURG inhibitors may interact with the enzyme in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the inhibitor binds to the enzyme.

A compound designed or selected as binding to MURG may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the inhibitor and the enzyme when the inhibitor is bound to MURG, preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include, but are not limited to: Gaussian 92, revision C [M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa. .COPYRIGHT.1992]; AMBER, version 4.0 [P. A. Kollman, University of California at San Francisco, .COPYRIGHT.1994]; QUANTA/CHARMM [Molecular Simulations, Inc., Burlington, Mass. .COPYRIGHT.1994]; and Insight II/Discover (Biosysm Technologies Inc., San Diego, Calif. .COPYRIGHT.1994). These programs may be implemented, for instance, using a Silicon Graphics workstation, IRIS Octane or IBM RISC/6000 workstation. Other hardware systems and software packages will be known to those skilled in the art.

Once a MurG-binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted

chemical compounds may then be analyzed for efficiency of fit to MURG by the same computer methods described in detail, above.

COMPOUNDS AND COMPOSITIONS COMPRISING COMPOUNDS DERIVED FROM STRUCTURE BASED DRUG DESIGN

One embodiment of the present invention is a compound that is capable of binding to a MurG protein, inhibiting the activity of a MurG protein, or stimulating the activity of a MurG protein. Suitable inhibitory compounds of the present invention can: (1) inhibit (i.e., prevent or block) the activity of MurG enzyme by binding to a MurG donor nucleotide binding site and interfering with the binding of the donor nucleotide molecule; (2) inhibit the activity of MurG enzyme by binding to the MurG acceptor binding site and interfering with the binding of the acceptor molecule; (3) inhibit the activity of a MurG enzyme by binding to the membrane association site and interfering with the association of the protein with the bacterial membrane and/or acceptor molecule.

Another embodiment of the present invention is a compound that is capable of stimulating MurG activity. Suitable stimulatory compounds of the present invention can stimulate the activity of a MurG enzyme by binding to the protein at a binding site and causing an increase in enzymatic activity, for example, by increasing the enzymes affinity to bind a donor nucleotide, an acceptor molecule or improve the enzymes stability or increasing the binding affinity of a molecule to MurG.

Such compounds that bind to, inhibit or stimulate activity of a MurG protein include, for example, compounds that mimic donor nucleotide molecules. In preferred embodiments, the compound includes, for example, pyrimidine nucleoside analogues. In yet another preferred embodiment, the compounds include compounds comprising a pyrimidine nucleoside with a substituent containing at least one heteroatom attached to the C5 hydroxyl. In more particular embodiments, pyrimidine derivatives make complementary hydrogen bonding contacts to the amide backbone segment containing Ile 245 and also contact glutamate 269.

Another embodiment of the present invention is a compound that binds to the acceptor binding site of the MurG protein, hereinafter referred to a acceptor analogs. An acceptor analog refers to a compound that interacts with (e.g., binds to, associates with, modifies) the acceptor binding site of a MurG protein. An acceptor analog, for example,

is a compound that mimics the natural acceptor molecule, Lipid I. Examples of such acceptor analogs are set forth in Ha et al., J. Amer. Chem. Soc. 1999, and PCT/US99/02187, U.S. Provisional Application No. 60/073,376 filed February 2, 1998, incorporated herein by reference.

Another embodiment of the present invention is a compound that binds to the MurG protein, that are enzyme product analogs, hereinafter referred to as Lipid II analogs. A Lipid II analog refers to a compound that interacts with (i.e. , binds to, associates with, modifies) the acceptor binding site of a Mur G protein which mimics the product of the transglycosylase reaction.

Inhibitory and stimulatory compounds of the present invention can be identified by various means known to those of skill in the art. For example, binding of an inhibitory compound to, or otherwise interaction with, a MurG protein, can be determined with MurG in solution, for example, using assays described in PCT/US99/02187, U.S. Provisional Application No. 60/073,376 filed February 2, 1998, and PCT/US00/05554 , U.S. Provisional Application Nos. 60/122,966 and 60/137,696, incorporated herein by reference.

According to the present invention, suitable compounds of the present invention include peptides or other organic molecules, and inorganic molecules. Suitable organic molecules include small organic molecules. Preferably, a compound of the present invention is not harmful (i.e., toxic) to an animal when administered to an animal.

Compounds of the present invention also can be identified using structure based drug design techniques known to those skilled in the art and described herein above.

Also according to the present invention, compounds are suitable for use in the inhibition of bacterial or microbial growth in an animal, and for example, function as an antibiotic for treatment of bacterial infections in animals.

The present invention also includes compositions comprising compounds of the present invention that inhibit or stimulate MurG activity which function as antibiotics or antimicrobial agents in animals. Compositions of the present invention can be used therapeutically or diagnostically in an animal. Compositions of the present invention comprises at least one compound of the present invention. In a preferred embodiment, compositions of the present invention further comprise a carrier. More particularly, a suitable carrier is a pharmaceutically acceptable carrier known to those skilled in the art.

TABLE 1- ATOMIC COORDINATES OF E. COLI MURG PROTEIN

REMARK coordinates from minimization refinementREMARK refinement
resolution: 40.0 - 1.9 AREMARK starting r= 0.2200 free_r= 0.2466REMARK
final   r= 0.2200 free_r= 0.2466REMARK rmsd bonds= 0.005558   rmsd
angles=   1.29505REMARK wa= 1.08391REMARK target= mlf cycles= 1 steps=
30REMARK sg= P1 a= 60.613 b= 66.356 c= 67.902 alpha= 64.294 beta=
83.520 gamma= 65.448REMARK parameter file 1 :
CNS_TOPPAR:protein_rep.paramREMARK parameter file 2 :
CNS_TOPPAR:water_rep.paramREMARK parameter file 3 :
CNS_TOPPAR:ion.paramREMARK molecular structure file: gen.mtfREMARK
input coordinates: gen.pdbREMARK reflection file= native.cvREMARK ncs=
noneREMARK B-correction resolution: 6.0 - 1.9REMARK initial B-factor
correction applied to fobs :REMARK   B11=   0.747 B22=   2.098 B33=   -
2.845REMARK   B12= -1.847 B13= -3.752 B23=   6.401REMARK B-factor
correction applied to coordinate array B: 0.038REMARK bulk solvent:
density level= 0.351665 e/A^3, B-factor= 43.8282 A^2REMARK reflections
with |Fobs|/sigma_F < 2.0 rejectedREMARK reflections with |Fobs| >
10000 * rms(Fobs) rejectedREMARK theoretical total number of refl. in
resol. range:68102 (100.0%)REMARK number of unobserved reflections (no
entry or |F|=0):2825(4.1%) REMARK number of reflections rejected:
3288 (4.8 %)REMARK total number of reflections used:
61989 91.0%)REMARK number of reflections in working set:
55765 (81.9%)REMARK number of reflections in test set:
6224 (9.1%)CRYST1   60.613   66.356   67.902 64.29 83.52 65.45 P 1
REMARK FILENAME="minimize5.pdb"REMARK DATE:14-Jan-00 15:25:36
created by user: shaREMARK VERSION:
0.5

ATOM	1	CB	LYS A	7	0.142	3.434	35.023	1.00	43.02	AAAA
ATOM	2	CG	LYS A	7	1.076	4.457	35.641	1.00	46.34	AAAA
ATOM	3	CD	LYS A	7	0.452	5.841	35.634	1.00	47.39	AAAA
ATOM	4	CE	LYS A	7	1.345	6.846	36.332	1.00	48.65	AAAA
ATOM	5	NZ	LYS A	7	0.780	8.221	36.276	1.00	51.04	AAAA
ATOM	6	C	LYS A	7	-2.239	2.733	34.833	1.00	39.64	AAAA
ATOM	7	O	LYS A	7	-2.050	1.717	34.160	1.00	39.64	AAAA
ATOM	8	N	LYS A	7	-0.974	2.320	36.947	1.00	42.05	AAAA
ATOM	9	CA	LYS A	7	-1.170	3.245	35.788	1.00	41.31	AAAA
ATOM	10	N	ARG A	8	-3.357	3.451	34.773	1.00	37.24	AAAA
ATOM	11	CA	ARG A	8	-4.469	3.076	33.906	1.00	34.91	AAAA
ATOM	12	CB	ARG A	8	-5.782	3.109	34.686	1.00	36.65	AAAA
ATOM	13	CG	ARG A	8	-5.950	2.017	35.721	1.00	39.89	AAAA
ATOM	14	CD	ARG A	8	-7.323	2.124	36.356	1.00	42.12	AAAA
ATOM	15	NE	ARG A	8	-7.663	0.960	37.163	1.00	45.03	AAAA
ATOM	16	CZ	ARG A	8	-7.031	0.610	38.279	1.00	46.29	AAAA
ATOM	17	NH1	ARG A	8	-6.015	1.337	38.725	1.00	46.88	AAAA
ATOM	18	NH2	ARG A	8	-7.420	-0.466	38.952	1.00	47.41	AAAA
ATOM	19	C	ARG A	8	-4.584	3.999	32.696	1.00	32.27	AAAA
ATOM	20	O	ARG A	8	-4.602	5.224	32.832	1.00	31.60	AAAA
ATOM	21	N	LEU A	9	-4.663	3.403	31.512	1.00	29.57	AAAA
ATOM	22	CA	LEU A	9	-4.792	4.171	30.283	1.00	27.45	AAAA
ATOM	23	CB	LEU A	9	-3.581	3.954	29.362	1.00	26.31	AAAA
ATOM	24	CG	LEU A	9	-3.752	4.466	27.916	1.00	25.77	AAAA
ATOM	25	CD1	LEU A	9	-3.670	5.985	27.895	1.00	24.31	AAAA

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ATOM     26  CD2 LEU A   9      -2.679   3.870  26.993  1.00 26.22      AAAA
ATOM     27  C   LEU A   9      -6.038   3.762  29.523  1.00 25.97      AAAA
ATOM     28  O   LEU A   9      -6.397   2.587  29.485  1.00 25.57      AAAA
ATOM     29  N   MET A  10      -6.713   4.738  28.928  1.00 25.37      AAAA
ATOM     30  CA  MET A  10      -7.866   4.429  28.101  1.00 24.70      AAAA
ATOM     31  CB  MET A  10      -9.142   5.101  28.612  1.00 25.60      AAAA
ATOM     32  CG  MET A  10     -10.323   4.873  27.675  1.00 25.77      AAAA
ATOM     33  SD  MET A  10     -11.916   4.958  28.492  1.00 26.63      AAAA
ATOM     34  CE  MET A  10     -12.197   3.222  28.862  1.00 25.72      AAAA
ATOM     35  C   MET A  10      -7.528   4.943  26.715  1.00 23.31      AAAA
ATOM     36  O   MET A  10      -7.198   6.116  26.544  1.00 24.02      AAAA
ATOM     37  N   VAL A  11      -7.574   4.059  25.727  1.00 22.25      AAAA
ATOM     38  CA  VAL A  11      -7.278   4.461  24.359  1.00 22.34      AAAA
ATOM     39  CB  VAL A  11      -6.444   3.386  23.624  1.00 22.75      AAAA
ATOM     40  CG1 VAL A  11      -6.256   3.768  22.158  1.00 20.51      AAAA
ATOM     41  CG2 VAL A  11      -5.082   3.239  24.310  1.00 21.75      AAAA
ATOM     42  C   VAL A  11      -8.612   4.654  23.646  1.00 22.94      AAAA
ATOM     43  O   VAL A  11      -9.525   3.843  23.804  1.00 23.37      AAAA
ATOM     44  N   MET A  12      -8.722   5.734  22.878  1.00 22.18      AAAA
ATOM     45  CA  MET A  12      -9.949   6.034  22.146  1.00 23.10      AAAA
ATOM     46  CB  MET A  12     -10.496   7.399  22.589  1.00 22.78      AAAA
ATOM     47  CG  MET A  12     -10.359   7.655  24.096  1.00 23.92      AAAA
ATOM     48  SD  MET A  12     -10.955   9.279  24.657  1.00 25.51      AAAA
ATOM     49  CE  MET A  12      -9.641  10.349  24.162  1.00 22.79      AAAA
ATOM     50  C   MET A  12      -9.582   6.072  20.673  1.00 22.97      AAAA
ATOM     51  O   MET A  12      -8.917   6.997  20.226  1.00 21.16      AAAA
ATOM     52  N   ALA A  13      -9.992   5.057  19.921  1.00 26.97      AAAA
ATOM     53  CA  ALA A  13      -9.665   5.008  18.498  1.00 30.88      AAAA
ATOM     54  CB  ALA A  13      -8.381   4.212  18.288  1.00 31.18      AAAA
ATOM     55  C   ALA A  13     -10.813   4.412  17.685  1.00 34.35      AAAA
ATOM     56  O   ALA A  13     -11.328   3.335  18.006  1.00 35.86      AAAA
ATOM     57  N   GLY A  14     -11.176   5.127  16.622  1.00 37.37      AAAA
ATOM     58  CA  GLY A  14     -12.287   4.762  15.757  1.00 40.54      AAAA
ATOM     59  C   GLY A  14     -12.239   3.583  14.808  1.00 41.52      AAAA
ATOM     60  O   GLY A  14     -11.267   2.831  14.755  1.00 43.26      AAAA
ATOM     61  N   GLY A  15     -13.322   3.451  14.042  1.00 42.70      AAAA
ATOM     62  CA  GLY A  15     -13.491   2.363  13.094  1.00 43.13      AAAA
ATOM     63  C   GLY A  15     -12.660   2.286  11.825  1.00 43.41      AAAA
ATOM     64  O   GLY A  15     -13.212   2.187  10.730  1.00 44.39      AAAA
ATOM     65  N   THR A  16     -11.340   2.333  11.966  1.00 43.38      AAAA
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ATOM	1173	CB	VAL A 163	7.182	1.224	11.417	1.00	31.04	AAAA
ATOM	1174	CG1	VAL A 163	7.571	0.308	10.260	1.00	30.44	AAAA
ATOM	1175	CG2	VAL A 163	6.902	2.631	10.914	1.00	29.10	AAAA
ATOM	1176	C	VAL A 163	6.258	-0.744	12.652	1.00	31.06	AAAA
ATOM	1177	O	VAL A 163	6.884	-0.892	13.706	1.00	29.66	AAAA
ATOM	1178	N	ARG A 164	5.820	-1.773	11.927	1.00	31.83	AAAA
ATOM	1179	CA	ARG A 164	6.124	-3.142	12.339	1.00	34.34	AAAA
ATOM	1180	CB	ARG A 164	5.533	-4.167	11.354	1.00	36.31	AAAA
ATOM	1181	CG	ARG A 164	5.704	-3.841	9.876	1.00	39.86	AAAA
ATOM	1182	CD	ARG A 164	4.855	-4.770	8.997	1.00	41.13	AAAA
ATOM	1183	NE	ARG A 164	5.368	-6.140	8.946	1.00	43.44	AAAA
ATOM	1184	CZ	ARG A 164	4.765	-7.145	8.311	1.00	44.08	AAAA
ATOM	1185	NH1	ARG A 164	3.619	-6.940	7.671	1.00	44.91	AAAA
ATOM	1186	NH2	ARG A 164	5.308	-8.355	8.308	1.00	44.44	AAAA
ATOM	1187	C	ARG A 164	7.649	-3.248	12.419	1.00	34.72	AAAA
ATOM	1188	O	ARG A 164	8.364	-2.769	11.537	1.00	33.63	AAAA
ATOM	1189	N	THR A 165	8.138	-3.855	13.496	1.00	34.72	AAAA
ATOM	1190	CA	THR A 165	9.567	-3.969	13.730	1.00	34.94	AAAA
ATOM	1191	CB	THR A 165	9.839	-4.437	15.177	1.00	35.90	AAAA
ATOM	1192	OG1	THR A 165	9.008	-5.563	15.488	1.00	36.96	AAAA
ATOM	1193	CG2	THR A 165	9.530	-3.313	16.149	1.00	35.88	AAAA
ATOM	1194	C	THR A 165	10.373	-4.814	12.749	1.00	34.61	AAAA
ATOM	1195	O	THR A 165	11.577	-4.603	12.608	1.00	34.56	AAAA
ATOM	1196	N	ASP A 166	9.739	-5.765	12.068	1.00	34.66	AAAA
ATOM	1197	CA	ASP A 166	10.492	-6.558	11.103	1.00	34.85	AAAA
ATOM	1198	CB	ASP A 166	9.697	-7.784	10.642	1.00	36.47	AAAA
ATOM	1199	CG	ASP A 166	8.341	-7.430	10.089	1.00	37.65	AAAA
ATOM	1200	OD1	ASP A 166	7.566	-8.365	9.804	1.00	41.03	AAAA
ATOM	1201	OD2	ASP A 166	8.048	-6.227	9.937	1.00	39.97	AAAA
ATOM	1202	C	ASP A 166	10.862	-5.667	9.917	1.00	33.70	AAAA
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ATOM	1206	CB	VAL A 167	9.096	-2.888	8.170	1.00	31.53	AAAA
ATOM	1207	CG1	VAL A 167	9.485	-1.738	7.248	1.00	30.83	AAAA
ATOM	1208	CG2	VAL A 167	8.120	-3.825	7.458	1.00	31.61	AAAA
ATOM	1209	C	VAL A 167	11.400	-2.657	9.108	1.00	31.23	AAAA
ATOM	1210	O	VAL A 167	12.320	-2.268	8.380	1.00	30.04	AAAA
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ATOM	1212	CA	LEU A 168	12.159	-1.277	10.959	1.00	32.61	AAAA
ATOM	1213	CB	LEU A 168	11.714	-0.942	12.387	1.00	33.77	AAAA

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ATOM	1215	CD1	LEU	A	168	10.141	0.076	14.041	1.00	35.50
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ATOM	1216	CD2	LEU	A	168	10.790	1.338	11.974	1.00	34.18
			AAAA							
ATOM	1217	C	LEU	A	168	13.594	-1.790	10.986	1.00	32.72
			AAAA							
ATOM	1218	O	LEU	A	168	14.538	-1.002	10.923	1.00	32.67
			AAAA							
ATOM	1219	N	ALA	A	169	13.752	-3.109	11.076	1.00	33.35
			AAAA							
ATOM	1220	CA	ALA	A	169	15.077	-3.725	11.138	1.00	34.36
			AAAA							
ATOM	1221	CB	ALA	A	169	14.992	-5.054	11.883	1.00	33.96
			AAAA							
ATOM	1222	C	ALA	A	169	15.746	-3.939	9.777	1.00	35.45
			AAAA							
ATOM	1223	O	ALA	A	169	16.905	-4.362	9.713	1.00	36.53
			AAAA							
ATOM	1224	N	LEU	A	170	15.030	-3.651	8.695	1.00	34.52
			AAAA							
ATOM	1225	CA	LEU	A	170	15.590	-3.833	7.358	1.00	34.60
			AAAA							
ATOM	1226	CB	LEU	A	170	14.577	-3.423	6.281	1.00	34.25
			AAAA							
ATOM	1227	CG	LEU	A	170	13.363	-4.333	6.071	1.00	33.98
			AAAA							
ATOM	1228	CD1	LEU	A	170	12.393	-3.675	5.101	1.00	34.11
			AAAA							
ATOM	1229	CD2	LEU	A	170	13.820	-5.688	5.543	1.00	33.52
			AAAA							
ATOM	1230	C	LEU	A	170	16.880	-3.042	7.163	1.00	34.41
			AAAA							
ATOM	1231	O	LEU	A	170	17.001	-1.902	7.616	1.00	33.45
			AAAA							
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			AAAA							
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			AAAA							
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			AAAA							
ATOM	1235	CB	PRO	A	171	19.897	-4.005	5.366	1.00	34.52
			AAAA							
ATOM	1236	CG	PRO	A	171	19.361	-5.308	5.844	1.00	34.60
			AAAA							
ATOM	1237	C	PRO	A	171	18.938	-1.665	5.503	1.00	35.39
			AAAA							
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			AAAA							
ATOM	1239	N	LEU	A	172	19.884	-0.746	5.654	1.00	36.05
			AAAA							
ATOM	1240	CA	LEU	A	172	19.801	0.555	4.998	1.00	37.43
			AAAA							
ATOM	1241	CB	LEU	A	172	20.946	1.458	5.468	1.00	37.48
			AAAA							
ATOM	1242	CG	LEU	A	172	20.934	1.934	6.925	1.00	38.42
			AAAA							
ATOM	1243	CD1	LEU	A	172	19.751	2.863	7.158	1.00	37.89
			AAAA							
ATOM	1244	CD2	LEU	A	172	20.876	0.735	7.859	1.00	38.70
			AAAA							
ATOM	1245	C	LEU	A	172	19.865	0.400	3.479	1.00	38.03
			AAAA							
ATOM	1246	O	LEU	A	172	20.392	-0.591	2.969	1.00	38.19
			AAAA							

ATOM	1247	N	PRO A 173	19.329	1.383	2.737	1.00	38.41	
ATOM	1248	CD	PRO A 173	18.647	2.586	3.248	1.00	38.12	
ATOM	1249	CA	PRO A 173	19.319	1.367	1.271	1.00	39.54	
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ATOM	1251	CG	PRO A 173	17.898	3.076	2.029	1.00	38.41	
ATOM	1252	C	PRO A 173	20.672	1.027	0.639	1.00	41.06	
ATOM	1253	O	PRO A 173	20.751	0.205	-0.276	1.00	41.26	
ATOM	1254	N	GLN A 174	21.734	1.659	1.127	1.00	42.31	
ATOM	1255	CA	GLN A 174	23.063	1.401	0.591	1.00	43.56	
ATOM	1256	CB	GLN A 174	24.118	2.219	1.343	1.00	45.08	
ATOM	1257	CG	GLN A 174	24.197	3.672	0.906	1.00	47.91	
ATOM	1258	CD	GLN A 174	25.366	4.413	1.534	1.00	50.04	
ATOM	1259	OE1	GLN A 174	25.665	5.552	1.164	1.00	50.92	
ATOM	1260	NE2	GLN A 174	26.033	3.771	2.491	1.00	50.23	
ATOM	1261	C	GLN A 174	23.415	-0.076	0.667	1.00	43.25	
ATOM	1262	O	GLN A 174	23.955	-0.641	-0.280	1.00	42.73	
ATOM	1263	N	GLN A 175	23.098	-0.702	1.794	1.00	43.02	
ATOM	1264	CA	GLN A 175	23.398	-2.115	1.981	1.00	43.41	
ATOM	1265	CB	GLN A 175	23.206	-2.505	3.449	1.00	44.88	
ATOM	1266	CG	GLN A 175	23.844	-1.544	4.444	1.00	47.91	
ATOM	1267	CD	GLN A 175	25.331	-1.344	4.211	1.00	49.82	
ATOM	1268	OE1	GLN A 175	25.747	-0.765	3.203	1.00	50.30	
ATOM	1269	NE2	GLN A 175	26.145	-1.826	5.148	1.00	51.04	
ATOM	1270	C	GLN A 175	22.521	-2.997	1.097	1.00	42.34	
ATOM	1271	O	GLN A 175	22.996	-3.961	0.500	1.00	41.64	
ATOM	1272	N	ARG A 176	21.238	-2.659	1.016	1.00	41.73	
ATOM	1273	CA	ARG A 176	20.285	-3.422	0.216	1.00	41.37	
ATOM	1274	CB	ARG A 176	18.854	-2.912	0.469	1.00	42.69	
ATOM	1275	CG	ARG A 176	17.767	-3.726	-0.232	1.00	44.32	
ATOM	1276	CD	ARG A 176	16.338	-3.227	0.066	1.00	46.28	
ATOM	1277	NE	ARG A 176	15.922	-2.116	-0.793	1.00	46.82	
ATOM	1278	CZ	ARG A 176	16.043	-0.829	-0.479	1.00	47.07	
ATOM	1279	NH1	ARG A 176	16.567	-0.471	0.686	1.00	47.74	

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ATOM    1296    N    GLY A 179      25.668   -3.299   -5.221   1.00 40.21
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ATOM	1334	CG1	VAL A 184	12.865	-0.901	-10.673	1.00	25.72
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ATOM	1335	CG2	VAL A 184	14.670	-0.648	-12.374	1.00	26.35
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ATOM	1341	CG	ARG A 185	13.910	-6.440	-8.323	1.00	25.75
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ATOM	1344	CZ	ARG A 185	16.784	-8.093	-6.623	1.00	29.19
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AAAA								

ATOM	1346	NH2	ARG	A	185	17.903	-8.679	-7.032	1.00	31.00
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AAAA										
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AAAA										
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AAAA										
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ATOM	1358	CB	LEU	A	187	6.979	-4.363	-4.379	1.00	22.77
AAAA										
ATOM	1359	CG	LEU	A	187	6.492	-5.359	-3.316	1.00	24.90
AAAA										
ATOM	1360	CD1	LEU	A	187	6.763	-4.768	-1.932	1.00	23.74
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AAAA										
ATOM	1362	C	LEU	A	187	5.104	-3.691	-5.871	1.00	21.37
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AAAA										
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ATOM	1365	CA	VAL	A	188	2.706	-3.774	-6.355	1.00	22.58
AAAA										
ATOM	1366	CB	VAL	A	188	1.988	-4.190	-7.657	1.00	22.95
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AAAA										
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AAAA										
ATOM	1370	O	VAL	A	188	1.603	-5.456	-5.051	1.00	22.38
AAAA										
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AAAA										
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AAAA										
ATOM	1378	N	GLY	A	190	-1.629	-3.955	-2.975	1.00	27.50
AAAA										

ATOM	1379	CA	GLY A 190	-3.007	-3.505	-2.966	1.00	30.27
AAAA								
ATOM	1380	C	GLY A 190	-3.720	-3.736	-1.641	1.00	32.15
AAAA								
ATOM	1381	O	GLY A 190	-4.896	-3.403	-1.499	1.00	32.00
AAAA								
ATOM	1382	N	GLY A 191	-3.016	-4.299	-0.664	1.00	32.97
AAAA								
ATOM	1383	CA	GLY A 191	-3.640	-4.550	0.624	1.00	34.29
AAAA								
ATOM	1384	C	GLY A 191	-4.507	-5.794	0.607	1.00	34.92
AAAA								
ATOM	1385	O	GLY A 191	-4.741	-6.388	-0.444	1.00	34.34
AAAA								
ATOM	1386	N	SER A 192	-4.996	-6.183	1.778	1.00	36.47
AAAA								
ATOM	1387	CA	SER A 192	-5.827	-7.377	1.910	1.00	38.39
AAAA								
ATOM	1388	CB	SER A 192	-6.389	-7.460	3.335	1.00	39.07
AAAA								
ATOM	1389	OG	SER A 192	-7.124	-6.291	3.658	1.00	41.25
AAAA								
ATOM	1390	C	SER A 192	-6.974	-7.472	0.903	1.00	38.69
AAAA								
ATOM	1391	O	SER A 192	-7.293	-8.557	0.410	1.00	38.58
AAAA								
ATOM	1392	N	GLN A 193	-7.599	-6.344	0.595	1.00	38.60
AAAA								
ATOM	1393	CA	GLN A 193	-8.715	-6.367	-0.339	1.00	39.91
AAAA								
ATOM	1394	CB	GLN A 193	-9.787	-5.367	0.110	1.00	41.97
AAAA								
ATOM	1395	CG	GLN A 193	-10.354	-5.679	1.497	1.00	43.94
AAAA								
ATOM	1396	CD	GLN A 193	-10.790	-7.135	1.640	1.00	45.71
AAAA								
ATOM	1397	OE1	GLN A 193	-11.677	-7.607	0.922	1.00	46.93
AAAA								
ATOM	1398	NE2	GLN A 193	-10.162	-7.853	2.567	1.00	45.80
AAAA								
ATOM	1399	C	GLN A 193	-8.298	-6.098	-1.781	1.00	39.31
AAAA								
ATOM	1400	O	GLN A 193	-9.076	-6.320	-2.708	1.00	39.52
AAAA								
ATOM	1401	N	GLY A 194	-7.064	-5.642	-1.961	1.00	38.40
AAAA								
ATOM	1402	CA	GLY A 194	-6.560	-5.358	-3.291	1.00	38.11
AAAA								
ATOM	1403	C	GLY A 194	-6.961	-3.987	-3.797	1.00	37.62
AAAA								
ATOM	1404	O	GLY A 194	-7.904	-3.382	-3.291	1.00	37.80
AAAA								
ATOM	1405	N	ALA A 195	-6.228	-3.489	-4.787	1.00	36.62
AAAA								
ATOM	1406	CA	ALA A 195	-6.513	-2.191	-5.387	1.00	36.35
AAAA								
ATOM	1407	CB	ALA A 195	-5.290	-1.291	-5.305	1.00	35.75
AAAA								
ATOM	1408	C	ALA A 195	-6.898	-2.437	-6.842	1.00	36.61
AAAA								
ATOM	1409	O	ALA A 195	-6.038	-2.519	-7.717	1.00	35.93
AAAA								
ATOM	1410	N	ARG A 196	-8.198	-2.566	-7.080	1.00	36.94
AAAA								
ATOM	1411	CA	ARG A 196	-8.741	-2.828	-8.412	1.00	38.03
AAAA								

ATOM	1412	CB	ARG A 196	-10.229	-2.466	-8.450	1.00	40.33
AAAA								
ATOM	1413	CG	ARG A 196	-10.526	-0.968	-8.375	1.00	44.08
AAAA								
ATOM	1414	CD	ARG A 196	-9.935	-0.306	-7.129	1.00	46.46
AAAA								
ATOM	1415	NE	ARG A 196	-10.381	-0.949	-5.894	1.00	48.33
AAAA								
ATOM	1416	CZ	ARG A 196	-10.199	-0.439	-4.682	1.00	48.85
AAAA								
ATOM	1417	NH1	ARG A 196	-9.581	0.725	-4.538	1.00	49.51
AAAA								
ATOM	1418	NH2	ARG A 196	-10.636	-1.093	-3.615	1.00	49.95
AAAA								
ATOM	1419	C	ARG A 196	-8.023	-2.120	-9.558	1.00	37.11
AAAA								
ATOM	1420	O	ARG A 196	-7.729	-2.736	-10.583	1.00	36.96
AAAA								
ATOM	1421	N	ILE A 197	-7.739	-0.834	-9.392	1.00	35.89
AAAA								
ATOM	1422	CA	ILE A 197	-7.071	-0.091	-10.448	1.00	35.67
AAAA								
ATOM	1423	CB	ILE A 197	-7.049	1.427	-10.161	1.00	36.70
AAAA								
ATOM	1424	CG2	ILE A 197	-6.221	1.726	-8.918	1.00	36.91
AAAA								
ATOM	1425	CG1	ILE A 197	-6.485	2.162	-11.381	1.00	36.95
AAAA								
ATOM	1426	CD1	ILE A 197	-6.529	3.661	-11.272	1.00	38.71
AAAA								
ATOM	1427	C	ILE A 197	-5.644	-0.580	-10.694	1.00	34.73
AAAA								
ATOM	1428	O	ILE A 197	-5.178	-0.575	-11.833	1.00	33.53
AAAA								
ATOM	1429	N	LEU A 198	-4.948	-0.992	-9.638	1.00	32.35
AAAA								
ATOM	1430	CA	LEU A 198	-3.588	-1.494	-9.813	1.00	31.48
AAAA								
ATOM	1431	CB	LEU A 198	-2.862	-1.633	-8.467	1.00	31.03
AAAA								
ATOM	1432	CG	LEU A 198	-2.548	-0.342	-7.704	1.00	32.00
AAAA								
ATOM	1433	CD1	LEU A 198	-1.773	-0.688	-6.442	1.00	30.82
AAAA								
ATOM	1434	CD2	LEU A 198	-1.734	0.607	-8.566	1.00	30.86
AAAA								
ATOM	1435	C	LEU A 198	-3.668	-2.850	-10.501	1.00	29.72
AAAA								
ATOM	1436	O	LEU A 198	-2.837	-3.173	-11.344	1.00	29.46
AAAA								
ATOM	1437	N	ASN A 199	-4.678	-3.639	-10.150	1.00	28.63
AAAA								
ATOM	1438	CA	ASN A 199	-4.848	-4.952	-10.758	1.00	28.66
AAAA								
ATOM	1439	CB	ASN A 199	-5.975	-5.724	-10.066	1.00	27.71
AAAA								
ATOM	1440	CG	ASN A 199	-5.641	-6.069	-8.632	1.00	26.12
AAAA								
ATOM	1441	OD1	ASN A 199	-4.501	-5.904	-8.200	1.00	24.15
AAAA								
ATOM	1442	ND2	ASN A 199	-6.631	-6.553	-7.884	1.00	24.90
AAAA								
ATOM	1443	C	ASN A 199	-5.144	-4.841	-12.248	1.00	29.87
AAAA								
ATOM	1444	O	ASN A 199	-4.834	-5.747	-13.024	1.00	30.26
AAAA								

ATOM	1445	N	GLN A 200	-5.746	-3.725	-12.644	1.00	31.15
AAAA								
ATOM	1446	CA	GLN A 200	-6.085	-3.498	-14.044	1.00	33.06
AAAA								
ATOM	1447	CB	GLN A 200	-7.396	-2.706	-14.145	1.00	34.24
AAAA								
ATOM	1448	CG	GLN A 200	-8.590	-3.368	-13.471	1.00	38.64
AAAA								
ATOM	1449	CD	GLN A 200	-8.923	-4.734	-14.050	1.00	41.05
AAAA								
ATOM	1450	OE1	GLN A 200	-9.131	-4.879	-15.256	1.00	43.10
AAAA								
ATOM	1451	NE2	GLN A 200	-8.983	-5.745	-13.185	1.00	43.12
AAAA								
ATOM	1452	C	GLN A 200	-4.989	-2.753	-14.812	1.00	32.52
AAAA								
ATOM	1453	O	GLN A 200	-4.809	-2.970	-16.008	1.00	34.23
AAAA								
ATOM	1454	N	THR A 201	-4.247	-1.895	-14.120	1.00	31.87
AAAA								
ATOM	1455	CA	THR A 201	-3.207	-1.092	-14.756	1.00	31.72
AAAA								
ATOM	1456	CB	THR A 201	-3.046	0.245	-13.999	1.00	32.41
AAAA								
ATOM	1457	OG1	THR A 201	-4.307	0.931	-13.976	1.00	32.19
AAAA								
ATOM	1458	CG2	THR A 201	-2.003	1.131	-14.668	1.00	32.29
AAAA								
ATOM	1459	C	THR A 201	-1.817	-1.728	-14.925	1.00	32.02
AAAA								
ATOM	1460	O	THR A 201	-1.206	-1.626	-15.991	1.00	31.47
AAAA								
ATOM	1461	N	MET A 202	-1.320	-2.394	-13.892	1.00	30.61
AAAA								
ATOM	1462	CA	MET A 202	0.019	-2.975	-13.963	1.00	30.10
AAAA								
ATOM	1463	CB	MET A 202	0.430	-3.507	-12.592	1.00	29.71
AAAA								
ATOM	1464	CG	MET A 202	0.564	-2.406	-11.548	1.00	28.99
AAAA								
ATOM	1465	SD	MET A 202	1.518	-0.961	-12.098	1.00	31.46
AAAA								
ATOM	1466	CE	MET A 202	3.184	-1.633	-12.184	1.00	29.20
AAAA								
ATOM	1467	C	MET A 202	0.286	-4.022	-15.042	1.00	29.48
AAAA								
ATOM	1468	O	MET A 202	1.389	-4.088	-15.568	1.00	29.15
AAAA								
ATOM	1469	N	PRO A 203	-0.703	-4.863	-15.379	1.00	30.34
AAAA								
ATOM	1470	CD	PRO A 203	-1.957	-5.186	-14.677	1.00	30.05
AAAA								
ATOM	1471	CA	PRO A 203	-0.415	-5.849	-16.426	1.00	31.11
AAAA								
ATOM	1472	CB	PRO A 203	-1.703	-6.654	-16.500	1.00	31.89
AAAA								
ATOM	1473	CG	PRO A 203	-2.188	-6.623	-15.072	1.00	31.09
AAAA								
ATOM	1474	C	PRO A 203	-0.103	-5.139	-17.746	1.00	33.02
AAAA								
ATOM	1475	O	PRO A 203	0.800	-5.530	-18.490	1.00	33.16
AAAA								
ATOM	1476	N	GLN A 204	-0.855	-4.081	-18.020	1.00	33.88
AAAA								
ATOM	1477	CA	GLN A 204	-0.666	-3.314	-19.242	1.00	34.99
AAAA								

ATOM	1478	CB	GLN A 204	-1.836	-2.347	-19.431	1.00	37.12
AAAA								
ATOM	1479	CG	GLN A 204	-3.177	-3.067	-19.538	1.00	40.86
AAAA								
ATOM	1480	CD	GLN A 204	-4.354	-2.121	-19.700	1.00	43.77
AAAA								
ATOM	1481	OE1	GLN A 204	-4.406	-1.330	-20.647	1.00	45.55
AAAA								
ATOM	1482	NE2	GLN A 204	-5.310	-2.198	-18.776	1.00	44.11
AAAA								
ATOM	1483	C	GLN A 204	0.659	-2.573	-19.190	1.00	33.42
AAAA								
ATOM	1484	O	GLN A 204	1.331	-2.431	-20.206	1.00	34.40
AAAA								
ATOM	1485	N	VAL A 205	1.045	-2.114	-18.002	1.00	32.44
AAAA								
ATOM	1486	CA	VAL A 205	2.313	-1.417	-17.836	1.00	30.42
AAAA								
ATOM	1487	CB	VAL A 205	2.466	-0.834	-16.408	1.00	31.72
AAAA								
ATOM	1488	CG1	VAL A 205	3.907	-0.406	-16.169	1.00	28.58
AAAA								
ATOM	1489	CG2	VAL A 205	1.544	0.356	-16.231	1.00	29.91
AAAA								
ATOM	1490	C	VAL A 205	3.446	-2.407	-18.086	1.00	30.65
AAAA								
ATOM	1491	O	VAL A 205	4.473	-2.062	-18.686	1.00	29.65
AAAA								
ATOM	1492	N	ALA A 206	3.255	-3.638	-17.616	1.00	29.08
AAAA								
ATOM	1493	CA	ALA A 206	4.253	-4.688	-17.796	1.00	30.43
AAAA								
ATOM	1494	CB	ALA A 206	3.763	-6.002	-17.169	1.00	27.77
AAAA								
ATOM	1495	C	ALA A 206	4.519	-4.886	-19.288	1.00	30.65
AAAA								
ATOM	1496	O	ALA A 206	5.668	-5.040	-19.709	1.00	30.70
AAAA								
ATOM	1497	N	ALA A 207	3.450	-4.879	-20.080	1.00	31.56
AAAA								
ATOM	1498	CA	ALA A 207	3.565	-5.053	-21.527	1.00	32.70
AAAA								
ATOM	1499	CB	ALA A 207	2.188	-4.997	-22.167	1.00	32.49
AAAA								
ATOM	1500	C	ALA A 207	4.470	-3.990	-22.145	1.00	32.72
AAAA								
ATOM	1501	O	ALA A 207	5.295	-4.284	-23.007	1.00	33.64
AAAA								
ATOM	1502	N	LYS A 208	4.321	-2.754	-21.692	1.00	33.07
AAAA								
ATOM	1503	CA	LYS A 208	5.112	-1.651	-22.216	1.00	33.20
AAAA								
ATOM	1504	CB	LYS A 208	4.477	-0.313	-21.814	1.00	35.14
AAAA								
ATOM	1505	CG	LYS A 208	3.199	0.044	-22.578	1.00	38.07
AAAA								
ATOM	1506	CD	LYS A 208	2.166	-1.062	-22.482	1.00	40.27
AAAA								
ATOM	1507	CE	LYS A 208	0.892	-0.731	-23.233	1.00	41.02
AAAA								
ATOM	1508	NZ	LYS A 208	-0.076	-1.857	-23.126	1.00	42.41
AAAA								
ATOM	1509	C	LYS A 208	6.571	-1.668	-21.779	1.00	32.58
AAAA								
ATOM	1510	O	LYS A 208	7.456	-1.274	-22.544	1.00	31.82
AAAA								

ATOM	1511	N	LEU	A	209	6.829	-2.121	-20.556	1.00	30.72
ATOM	1512	CA	LEU	A	209	8.193	-2.143	-20.042	1.00	30.48
ATOM	1513	CB	LEU	A	209	8.191	-1.848	-18.535	1.00	29.34
ATOM	1514	CG	LEU	A	209	7.596	-0.498	-18.107	1.00	31.02
ATOM	1515	CD1	LEU	A	209	7.779	-0.318	-16.605	1.00	29.42
ATOM	1516	CD2	LEU	A	209	8.273	0.641	-18.859	1.00	31.39
ATOM	1517	C	LEU	A	209	8.970	-3.432	-20.315	1.00	29.73
ATOM	1518	O	LEU	A	209	10.191	-3.455	-20.174	1.00	31.33
ATOM	1519	N	GLY	A	210	8.269	-4.494	-20.698	1.00	29.76
ATOM	1520	CA	GLY	A	210	8.924	-5.762	-20.986	1.00	29.99
ATOM	1521	C	GLY	A	210	10.007	-6.188	-20.003	1.00	30.99
ATOM	1522	O	GLY	A	210	9.788	-6.183	-18.789	1.00	30.80
ATOM	1523	N	ASP	A	211	11.181	-6.536	-20.535	1.00	30.05
ATOM	1524	CA	ASP	A	211	12.332	-6.999	-19.749	1.00	29.42
ATOM	1525	CB	ASP	A	211	13.466	-7.479	-20.676	1.00	30.83
ATOM	1526	CG	ASP	A	211	13.119	-8.735	-21.449	1.00	32.09
ATOM	1527	OD1	ASP	A	211	13.977	-9.193	-22.235	1.00	34.13
ATOM	1528	OD2	ASP	A	211	12.005	-9.269	-21.283	1.00	32.72
ATOM	1529	C	ASP	A	211	12.960	-6.011	-18.776	1.00	29.03
ATOM	1530	O	ASP	A	211	13.781	-6.417	-17.945	1.00	27.69
ATOM	1531	N	SER	A	212	12.613	-4.730	-18.876	1.00	28.54
ATOM	1532	CA	SER	A	212	13.204	-3.719	-18.002	1.00	27.61
ATOM	1533	CB	SER	A	212	12.927	-2.308	-18.538	1.00	28.62
ATOM	1534	OG	SER	A	212	11.546	-1.990	-18.498	1.00	30.84
ATOM	1535	C	SER	A	212	12.759	-3.805	-16.542	1.00	26.31
ATOM	1536	O	SER	A	212	13.395	-3.219	-15.666	1.00	25.39
ATOM	1537	N	VAL	A	213	11.675	-4.528	-16.284	1.00	25.65
ATOM	1538	CA	VAL	A	213	11.187	-4.671	-14.914	1.00	24.52
ATOM	1539	CB	VAL	A	213	9.967	-3.747	-14.621	1.00	25.58
ATOM	1540	CG1	VAL	A	213	10.296	-2.298	-14.953	1.00	26.31
ATOM	1541	CG2	VAL	A	213	8.758	-4.225	-15.394	1.00	25.15
ATOM	1542	C	VAL	A	213	10.751	-6.095	-14.607	1.00	23.77
ATOM	1543	O	VAL	A	213	10.427	-6.874	-15.506	1.00	23.79

ATOM	1544	N	THR A 214	10.770	-6.432	-13.323	1.00	23.49
ATOM	1545	CA	THR A 214	10.326	-7.735	-12.861	1.00	21.50
ATOM	1546	CB	THR A 214	11.499	-8.600	-12.325	1.00	21.99
ATOM	1547	OG1	THR A 214	10.987	-9.870	-11.909	1.00	23.56
ATOM	1548	CG2	THR A 214	12.220	-7.921	-11.174	1.00	20.60
ATOM	1549	C	THR A 214	9.342	-7.362	-11.760	1.00	21.46
ATOM	1550	O	THR A 214	9.657	-6.567	-10.880	1.00	21.12
ATOM	1551	N	ILE A 215	8.150	-7.938	-11.827	1.00	21.73
ATOM	1552	CA	ILE A 215	7.083	-7.601	-10.894	1.00	22.01
ATOM	1553	CB	ILE A 215	5.831	-7.139	-11.688	1.00	22.41
ATOM	1554	CG2	ILE A 215	4.707	-6.738	-10.734	1.00	22.94
ATOM	1555	CG1	ILE A 215	6.198	-5.964	-12.599	1.00	22.71
ATOM	1556	CD1	ILE A 215	5.078	-5.560	-13.545	1.00	21.71
ATOM	1557	C	ILE A 215	6.617	-8.685	-9.929	1.00	21.67
ATOM	1558	O	ILE A 215	6.600	-9.868	-10.257	1.00	20.14
ATOM	1559	N	TRP A 216	6.248	-8.247	-8.728	1.00	21.03
ATOM	1560	CA	TRP A 216	5.677	-9.121	-7.708	1.00	21.08
ATOM	1561	CB	TRP A 216	6.541	-9.186	-6.455	1.00	21.14
ATOM	1562	CG	TRP A 216	5.941	-10.063	-5.370	1.00	21.49
ATOM	1563	CD2	TRP A 216	6.624	-10.588	-4.226	1.00	21.97
ATOM	1564	CE2	TRP A 216	5.674	-11.309	-3.461	1.00	22.67
ATOM	1565	CE3	TRP A 216	7.947	-10.521	-3.773	1.00	22.25
ATOM	1566	CD1	TRP A 216	4.639	-10.478	-5.262	1.00	21.72
ATOM	1567	NE1	TRP A 216	4.472	-11.231	-4.112	1.00	22.34
ATOM	1568	CZ2	TRP A 216	6.011	-11.955	-2.265	1.00	24.81
ATOM	1569	CZ3	TRP A 216	8.283	-11.166	-2.582	1.00	23.37
ATOM	1570	CH2	TRP A 216	7.316	-11.872	-1.843	1.00	23.19
ATOM	1571	C	TRP A 216	4.401	-8.352	-7.396	1.00	21.75
ATOM	1572	O	TRP A 216	4.442	-7.330	-6.719	1.00	22.71
ATOM	1573	N	HIS A 217	3.280	-8.844	-7.909	1.00	23.00
ATOM	1574	CA	HIS A 217	1.987	-8.185	-7.751	1.00	24.05
ATOM	1575	CB	HIS A 217	1.301	-8.167	-9.127	1.00	25.31
ATOM	1576	CG	HIS A 217	0.075	-7.312	-9.201	1.00	27.29

ATOM	1577	CD2	HIS	A	217	-1.008	-7.226	-8.391	1.00 27.56
ATOM	1578	ND1	HIS	A	217	-0.146	-6.424	-10.233	1.00 28.22
ATOM	1579	CE1	HIS	A	217	-1.311	-5.828	-10.057	1.00 28.76
ATOM	1580	NE2	HIS	A	217	-1.856	-6.296	-8.947	1.00 27.39
ATOM	1581	C	HIS	A	217	1.095	-8.880	-6.714	1.00 22.49
ATOM	1582	O	HIS	A	217	0.785	-10.059	-6.851	1.00 24.60
ATOM	1583	N	GLN	A	218	0.696	-8.144	-5.679	1.00 24.33
ATOM	1584	CA	GLN	A	218	-0.184	-8.676	-4.629	1.00 24.84
ATOM	1585	CB	GLN	A	218	0.271	-8.181	-3.250	1.00 25.16
ATOM	1586	CG	GLN	A	218	-0.572	-8.709	-2.084	1.00 26.40
ATOM	1587	CD	GLN	A	218	-1.629	-7.722	-1.608	1.00 27.63
ATOM	1588	OE1	GLN	A	218	-2.762	-8.107	-1.297	1.00 29.31
ATOM	1589	NE2	GLN	A	218	-1.260	-6.455	-1.525	1.00 24.88
ATOM	1590	C	GLN	A	218	-1.573	-8.134	-4.983	1.00 24.83
ATOM	1591	O	GLN	A	218	-1.859	-6.960	-4.767	1.00 24.21
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ATOM	1594	CB	SER	A	219	-4.189	-9.704	-7.035	1.00 28.46
ATOM	1595	OG	SER	A	219	-4.394	-10.949	-6.387	1.00 29.92
ATOM	1596	C	SER	A	219	-4.887	-8.470	-5.034	1.00 29.52
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ATOM	1598	N	GLY	A	220	-4.806	-9.135	-3.890	1.00 30.25
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ATOM	1600	C	GLY	A	220	-6.696	-10.302	-2.952	1.00 32.52
ATOM	1601	O	GLY	A	220	-6.554	-11.126	-3.862	1.00 31.13
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ATOM	1603	CA	LYS	A	221	-8.423	-11.619	-1.815	1.00 34.69
ATOM	1604	CB	LYS	A	221	-9.340	-11.421	-0.601	1.00 35.93
ATOM	1605	CG	LYS	A	221	-10.257	-12.593	-0.285	1.00 38.70
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ATOM	1607	CE	LYS	A	221	-11.955	-13.465	1.368	1.00 41.74
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ATOM	1609	C	LYS	A	221	-9.269	-11.932	-3.046	1.00 34.22

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ATOM	1680	CE1	TYR A 231	1.926	-7.786	-14.520	1.00	22.17
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ATOM	1701	N	ALA A 234	-1.093	-10.185	-21.398	1.00	30.89
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ATOM AAAA	1809	OD2	ASP	A	247	9.277	-12.816	5.791	1.00 32.31
ATOM AAAA	1810	C	ASP	A	247	6.422	-9.949	4.275	1.00 34.18
ATOM AAAA	1811	O	ASP	A	247	7.241	-10.003	3.354	1.00 33.62
ATOM AAAA	1812	N	MET	A	248	5.801	-8.825	4.617	1.00 33.66
ATOM AAAA	1813	CA	MET	A	248	6.069	-7.577	3.916	1.00 33.29
ATOM AAAA	1814	CB	MET	A	248	5.192	-6.448	4.461	1.00 34.30
ATOM AAAA	1815	CG	MET	A	248	3.852	-6.314	3.757	1.00 36.70
ATOM AAAA	1816	SD	MET	A	248	4.042	-5.940	1.987	1.00 40.22
ATOM AAAA	1817	CE	MET	A	248	2.590	-6.667	1.361	1.00 39.66
ATOM AAAA	1818	C	MET	A	248	7.533	-7.180	4.017	1.00 32.64
ATOM AAAA	1819	O	MET	A	248	8.082	-6.587	3.088	1.00 32.59
ATOM AAAA	1820	N	ALA	A	249	8.166	-7.500	5.142	1.00 30.31
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ATOM AAAA	1822	CB	ALA	A	249	10.061	-7.597	6.706	1.00 28.83
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ATOM AAAA	1835	N	TYR	A	252	9.832	-6.097	0.855	1.00 24.41
ATOM AAAA	1836	CA	TYR	A	252	10.488	-4.801	0.838	1.00 24.62
ATOM AAAA	1837	CB	TYR	A	252	10.191	-4.033	2.131	1.00 26.30
ATOM AAAA	1838	CG	TYR	A	252	8.815	-3.399	2.214	1.00 28.84
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ATOM	1903	SG	CYS A 260	2.509	1.742	-1.683	1.00	29.42
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ATOM AAAA	1908	CB	ARG A 261	-3.244	2.848	-1.340	1.00	31.35
ATOM AAAA	1909	CG	ARG A 261	-4.237	2.168	-2.258	1.00	33.82
ATOM AAAA	1910	CD	ARG A 261	-4.829	3.143	-3.253	1.00	35.21
ATOM AAAA	1911	NE	ARG A 261	-5.949	2.547	-3.975	1.00	36.21
ATOM AAAA	1912	CZ	ARG A 261	-6.550	3.107	-5.017	1.00	36.46
ATOM AAAA	1913	NH1	ARG A 261	-6.138	4.283	-5.470	1.00	36.95
ATOM AAAA	1914	NH2	ARG A 261	-7.571	2.493	-5.599	1.00	37.72
ATOM AAAA	1915	C	ARG A 261	-1.118	4.076	-0.979	1.00	30.75
ATOM AAAA	1916	O	ARG A 261	-0.041	3.575	-0.641	1.00	29.94
ATOM AAAA	1917	N	SER A 262	-1.583	5.206	-0.453	1.00	30.70
ATOM AAAA	1918	CA	SER A 262	-0.807	5.924	0.544	1.00	31.00
ATOM AAAA	1919	CB	SER A 262	-0.290	7.245	-0.034	1.00	31.31
ATOM AAAA	1920	OG	SER A 262	-1.344	8.016	-0.581	1.00	32.21
ATOM AAAA	1921	C	SER A 262	-1.526	6.182	1.868	1.00	30.92
ATOM AAAA	1922	O	SER A 262	-1.624	7.322	2.317	1.00	31.37
ATOM AAAA	1923	N	GLY A 263	-2.040	5.121	2.483	1.00	30.70
ATOM AAAA	1924	CA	GLY A 263	-2.669	5.277	3.779	1.00	29.85
ATOM AAAA	1925	C	GLY A 263	-1.510	5.663	4.680	1.00	29.40
ATOM AAAA	1926	O	GLY A 263	-0.367	5.287	4.394	1.00	28.65
ATOM AAAA	1927	N	ALA A 264	-1.787	6.404	5.751	1.00	28.11
ATOM AAAA	1928	CA	ALA A 264	-0.752	6.872	6.674	1.00	28.19
ATOM AAAA	1929	CB	ALA A 264	-1.399	7.563	7.879	1.00	27.89
ATOM AAAA	1930	C	ALA A 264	0.249	5.826	7.166	1.00	27.95
ATOM AAAA	1931	O	ALA A 264	1.454	6.056	7.117	1.00	28.65
ATOM AAAA	1932	N	LEU A 265	-0.239	4.693	7.656	1.00	27.93
ATOM AAAA	1933	CA	LEU A 265	0.662	3.659	8.158	1.00	27.76
ATOM AAAA	1934	CB	LEU A 265	-0.141	2.524	8.798	1.00	28.60
ATOM AAAA	1935	CG	LEU A 265	-1.049	2.984	9.947	1.00	29.56
ATOM AAAA	1936	CD1	LEU A 265	-1.680	1.775	10.615	1.00	28.94
ATOM AAAA	1937	CD2	LEU A 265	-0.245	3.797	10.957	1.00	29.94
ATOM AAAA	1938	C	LEU A 265	1.566	3.116	7.053	1.00	27.53
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ATOM  1970  CA  ILE A 270      7.711   2.763   3.158  1.00 28.64
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ATOM  1971  CB  ILE A 270      6.968   3.520   2.028  1.00 28.20
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ATOM	1975	C	ILE	A	270	8.978	3.532	3.522	1.00	28.84
ATOM	1976	O	ILE	A	270	10.076	3.194	3.075	1.00	28.96
ATOM	1977	N	ALA	A	271	8.818	4.568	4.340	1.00	28.51
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ATOM	1979	CB	ALA	A	271	9.462	6.576	5.572	1.00	28.12
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ATOM	1982	N	ALA	A	272	10.370	3.755	6.534	1.00	28.79
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ATOM	1993	CA	GLY	A	274	13.937	3.078	2.814	1.00	32.26
ATOM	1994	C	GLY	A	274	13.725	2.683	1.362	1.00	32.80
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ATOM	1996	N	LEU	A	275	12.501	2.862	0.873	1.00	32.88
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ATOM	1998	CB	LEU	A	275	11.266	1.262	-0.502	1.00	32.79
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ATOM	2000	CD1	LEU	A	275	10.762	-1.133	-0.114	1.00	33.69
ATOM	2001	CD2	LEU	A	275	12.538	-0.484	-1.762	1.00	32.25
ATOM	2002	C	LEU	A	275	11.479	3.568	-1.324	1.00	33.39
ATOM	2003	O	LEU	A	275	10.638	4.320	-0.819	1.00	32.48
ATOM	2004	N	PRO	A	276	11.835	3.654	-2.617	1.00	32.76
ATOM	2005	CD	PRO	A	276	13.022	3.048	-3.244	1.00	32.59

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ATOM	2235	CB	ILE A 304	1.808	11.961	-5.492	1.00	42.27
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ATOM	2236	CG2	ILE A 304	0.321	11.738	-5.278	1.00	41.77
AAAA								

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AAAAATOM   2278  CD  GLN A 309     -1.077  13.975 -12.843  1.00 61.96
AAAAATOM   2279  OE1 GLN A 309     -0.180  13.974 -11.997  1.00 62.79
AAAAATOM   2280  NE2 GLN A 309     -1.226  14.956 -13.728  1.00 62.49
AAAAATOM   2281  C   GLN A 309     -3.250  10.459 -14.204  1.00 57.53
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AAAAATOM   2285  CB  LEU A 310     -3.799   7.473 -12.241  1.00 53.77
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AAAAATOM	2286	CG	LEU	A	310	-3.242	6.108	-11.804	1.00	53.75
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AAAAATOM	2298	CA	VAL	A	312	-1.056	2.972	-18.103	1.00	43.52
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AAAAATOM	2303	O	VAL	A	312	1.284	3.488	-17.922	1.00	41.92
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AAAAATOM	2309	OD2	ASP	A	313	-0.610	5.514	-22.896	1.00	48.38
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AAAAATOM	2317	N	VAL	A	315	1.940	5.648	-15.569	1.00	34.29
AAAAATOM	2318	CA	VAL	A	315	2.708	4.809	-14.652	1.00	33.44
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AAAAATOM	2323	O	VAL	A	315	5.071	4.426	-14.792	1.00	32.35
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AAAAATOM	2340	OG1	THR	A	318	5.353	8.460	-13.498	1.00	34.46
AAAAATOM	2341	CG2	THR	A	318	6.984	7.568	-11.969	1.00	34.42
AAAAATOM	2342	C	THR	A	318	8.335	6.252	-14.093	1.00	34.52
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AAAAATOM   2368   CD1  TRP A 322     12.126    8.091 -11.389   1.00 39.97
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AAAAATOM   2394   CB   GLU A 325     22.208    6.236 -10.304   1.00 42.74
AAAAATOM   2395   CG   GLU A 325     22.642    7.589  -9.745   1.00 46.19
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AAAAATOM   2402   CA   THR A 326     18.130    7.591  -9.102   1.00 40.25
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AAAAATOM   2446   CB   GLU A 332      19.470    7.607    0.465   1.00 44.04
AAAAATOM   2447   CG   GLU A 332      20.414    6.500    0.016   1.00 46.55
AAAAATOM   2448   CD   GLU A 332      21.822    6.994   -0.248   1.00 48.04
AAAAATOM   2449   OE1  GLU A 332      21.981    7.923   -1.065   1.00 49.87
AAAAATOM   2450   OE2  GLU A 332      22.770    6.449    0.359   1.00 49.38
AAAAATOM   2451   C    GLU A 332      17.246    8.228    1.445   1.00 42.38
AAAAATOM   2452   O    GLU A 332      17.156    8.435    2.653   1.00 42.66
AAAAATOM   2453   N    ARG A 333      16.619    8.969    0.540   1.00 41.80
AAAAATOM   2454   CA   ARG A 333      15.752   10.067    0.937   1.00 42.25
AAAAATOM   2455   CB   ARG A 333      15.212   10.784   -0.306   1.00 43.43
AAAAATOM   2456   CG   ARG A 333      16.184   11.793   -0.926   1.00 45.99
AAAAATOM   2457   CD   ARG A 333      15.844   12.060   -2.389   1.00 48.51
AAAAATOM   2458   NE   ARG A 333      16.415   13.301   -2.913   1.00 50.45
AAAAATOM   2459   CZ   ARG A 333      17.703   13.631   -2.859   1.00 52.07
AAAAATOM   2460   NH1  ARG A 333      18.585   12.814   -2.297   1.00 52.45
AAAAATOM   2461   NH2  ARG A 333      18.112   14.784   -3.377   1.00 51.94
AAAAATOM   2462   C    ARG A 333      14.594    9.519    1.777   1.00 41.39
AAAAATOM   2463   O    ARG A 333      14.275   10.060    2.834   1.00 40.21
AAAAATOM   2464   N    ALA A 334      13.981    8.435    1.308   1.00 40.03
AAAAATOM   2465   CA   ALA A 334      12.859    7.825    2.014   1.00 39.84
AAAAATOM   2466   CB   ALA A 334      12.356    6.612    1.241   1.00 38.43
AAAAATOM   2467   C    ALA A 334      13.239    7.417    3.435   1.00 40.05
AAAAATOM   2468   O    ALA A 334      12.493    7.665    4.386   1.00 40.41
AAAAATOM   2469   N    ARG A 335      14.404    6.797    3.577   1.00 39.11
AAAAATOM   2470   CA   ARG A 335      14.874    6.351    4.881   1.00 40.00
AAAAATOM   2471   CB   ARG A 335      16.137    5.506    4.719   1.00 39.98
AAAAATOM   2472   CG   ARG A 335      16.631    4.865    6.000   1.00 40.54
AAAAATOM   2473   CD   ARG A 335      15.653    3.814    6.501   1.00 42.08
AAAAATOM   2474   NE   ARG A 335      16.263    2.949    7.507   1.00 42.95
AAAAATOM   2475   CZ   ARG A 335      16.403    1.634    7.373   1.00 43.43
AAAAATOM   2476   NH1  ARG A 335      15.972    1.024    6.274   1.00 43.17
AAAAATOM   2477   NH2  ARG A 335      16.983    0.927    8.335   1.00 43.96
AAAAATOM   2478   C    ARG A 335      15.167    7.527    5.802   1.00 40.09
AAAAATOM   2479   O    ARG A 335      14.877    7.479    6.997   1.00 39.35
AAAAATOM   2480   N    ALA A 336      15.745    8.581    5.237   1.00 40.52
AAAAATOM   2481   CA   ALA A 336      16.089    9.774    6.001   1.00 41.50
AAAAATOM   2482   CB   ALA A 336      16.850   10.754    5.116   1.00 41.05
AAAAATOM   2483   C    ALA A 336      14.847   10.447    6.573   1.00 42.00
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AAAAATOM	2484	O	ALA A 336	14.905	11.087	7.621	1.00	42.49
AAAAATOM	2485	N	ALA A 337	13.725	10.300	5.879	1.00	42.58
AAAAATOM	2486	CA	ALA A 337	12.475	10.903	6.320	1.00	42.55
AAAAATOM	2487	CB	ALA A 337	11.656	11.338	5.111	1.00	42.34
AAAAATOM	2488	C	ALA A 337	11.670	9.932	7.174	1.00	42.43
AAAAATOM	2489	O	ALA A 337	10.444	10.000	7.209	1.00	44.01
AAAAATOM	2490	N	SER A 338	12.360	9.035	7.868	1.00	41.93
AAAAATOM	2491	CA	SER A 338	11.686	8.053	8.708	1.00	41.12
AAAAATOM	2492	CB	SER A 338	12.097	6.641	8.293	1.00	40.73
AAAAATOM	2493	OG	SER A 338	11.504	5.671	9.139	1.00	40.32
AAAAATOM	2494	C	SER A 338	11.964	8.235	10.198	1.00	40.88
AAAAATOM	2495	O	SER A 338	13.042	8.674	10.594	1.00	41.46
AAAAATOM	2496	N	ILE A 339	10.971	7.898	11.013	1.00	40.11
AAAAATOM	2497	CA	ILE A 339	11.080	7.985	12.461	1.00	39.66
AAAAATOM	2498	CB	ILE A 339	10.061	8.992	13.038	1.00	39.74
AAAAATOM	2499	CG2	ILE A 339	10.249	9.118	14.544	1.00	38.88
AAAAATOM	2500	CG1	ILE A 339	10.249	10.354	12.361	1.00	39.75
AAAAATOM	2501	CD1	ILE A 339	9.263	11.423	12.804	1.00	40.42
AAAAATOM	2502	C	ILE A 339	10.788	6.576	12.978	1.00	40.19
AAAAATOM	2503	O	ILE A 339	9.653	6.102	12.923	1.00	39.97
AAAAATOM	2504	N	PRO A 340	11.821	5.886	13.484	1.00	40.75
AAAAATOM	2505	CD	PRO A 340	13.225	6.336	13.448	1.00	40.95
AAAAATOM	2506	CA	PRO A 340	11.728	4.520	14.012	1.00	40.57
AAAAATOM	2507	CB	PRO A 340	13.161	4.021	13.877	1.00	41.22
AAAAATOM	2508	CG	PRO A 340	13.944	5.244	14.222	1.00	41.12
AAAAATOM	2509	C	PRO A 340	11.180	4.294	15.424	1.00	40.38
AAAAATOM	2510	O	PRO A 340	10.841	3.163	15.776	1.00	40.48
AAAAATOM	2511	N	ASP A 341	11.080	5.345	16.232	1.00	39.43
AAAAATOM	2512	CA	ASP A 341	10.603	5.174	17.603	1.00	38.32
AAAAATOM	2513	CB	ASP A 341	11.668	5.696	18.578	1.00	38.62
AAAAATOM	2514	CG	ASP A 341	12.044	7.146	18.317	1.00	39.54
AAAAATOM	2515	OD1	ASP A 341	11.727	7.658	17.221	1.00	38.30
AAAAATOM	2516	OD2	ASP A 341	12.668	7.771	19.209	1.00	40.07
AAAAATOM	2517	C	ASP A 341	9.241	5.789	17.939	1.00	37.27
AAAAATOM	2518	O	ASP A 341	9.014	6.235	19.066	1.00	35.88
AAAAATOM	2519	N	ALA A 342	8.329	5.789	16.971	1.00	36.20
AAAAATOM	2520	CA	ALA A 342	6.996	6.349	17.181	1.00	34.98
AAAAATOM	2521	CB	ALA A 342	6.150	6.156	15.927	1.00	35.84
AAAAATOM	2522	C	ALA A 342	6.280	5.744	18.389	1.00	34.17
AAAAATOM	2523	O	ALA A 342	5.843	6.465	19.289	1.00	33.36
AAAAATOM	2524	N	THR A 343	6.159	4.421	18.410	1.00	33.49
AAAAATOM	2525	CA	THR A 343	5.481	3.747	19.512	1.00	33.39
AAAAATOM	2526	CB	THR A 343	5.567	2.211	19.362	1.00	33.34
AAAAATOM	2527	OG1	THR A 343	4.951	1.818	18.128	1.00	34.05
AAAAATOM	2528	CG2	THR A 343	4.851	1.519	20.516	1.00	33.82
AAAAATOM	2529	C	THR A 343	6.067	4.155	20.865	1.00	33.89
AAAAATOM	2530	O	THR A 343	5.340	4.591	21.756	1.00	32.15
AAAAATOM	2531	N	GLU A 344	7.383	4.027	21.007	1.00	34.87
AAAAATOM	2532	CA	GLU A 344	8.055	4.379	22.257	1.00	35.80
AAAAATOM	2533	CB	GLU A 344	9.553	4.054	22.177	1.00	37.79
AAAAATOM	2534	CG	GLU A 344	9.892	2.570	22.029	1.00	41.45
AAAAATOM	2535	CD	GLU A 344	9.963	2.101	20.581	1.00	44.16
AAAAATOM	2536	OE1	GLU A 344	10.311	0.917	20.357	1.00	45.57
AAAAATOM	2537	OE2	GLU A 344	9.676	2.910	19.668	1.00	45.28
AAAAATOM	2538	C	GLU A 344	7.886	5.856	22.590	1.00	35.95
AAAAATOM	2539	O	GLU A 344	7.751	6.233	23.754	1.00	35.12
AAAAATOM	2540	N	ARG A 345	7.896	6.689	21.559	1.00	35.83
AAAAATOM	2541	CA	ARG A 345	7.759	8.127	21.731	1.00	36.32
AAAAATOM	2542	CB	ARG A 345	7.999	8.803	20.386	1.00	38.26
AAAAATOM	2543	CG	ARG A 345	8.268	10.280	20.448	1.00	41.85
AAAAATOM	2544	CD	ARG A 345	9.006	10.686	19.194	1.00	44.45
AAAAATOM	2545	NE	ARG A 345	9.194	12.128	19.098	1.00	47.27
AAAAATOM	2546	CZ	ARG A 345	9.855	12.721	18.111	1.00	47.66
AAAAATOM	2547	NH1	ARG A 345	10.390	11.988	17.144	1.00	48.37
AAAAATOM	2548	NH2	ARG A 345	9.974	14.042	18.090	1.00	48.27
AAAAATOM	2549	C	ARG A 345	6.384	8.510	22.289	1.00	35.99

AAAAATOM	2550	O	ARG	A	345	6.285	9.209	23.302	1.00 35.24
AAAAATOM	2551	N	VAL	A	346	5.324	8.052	21.630	1.00 34.14
AAAAATOM	2552	CA	VAL	A	346	3.975	8.355	22.092	1.00 33.40
AAAAATOM	2553	CB	VAL	A	346	2.909	7.816	21.110	1.00 33.26
AAAAATOM	2554	CG1	VAL	A	346	1.516	7.969	21.709	1.00 33.83
AAAAATOM	2555	CG2	VAL	A	346	3.005	8.565	19.793	1.00 32.47
AAAAATOM	2556	C	VAL	A	346	3.770	7.727	23.466	1.00 33.14
AAAAATOM	2557	O	VAL	A	346	3.172	8.336	24.352	1.00 32.24
AAAAATOM	2558	N	ALA	A	347	4.280	6.510	23.643	1.00 32.01
AAAAATOM	2559	CA	ALA	A	347	4.159	5.813	24.917	1.00 32.80
AAAAATOM	2560	CB	ALA	A	347	4.831	4.447	24.839	1.00 31.97
AAAAATOM	2561	C	ALA	A	347	4.788	6.639	26.031	1.00 33.01
AAAAATOM	2562	O	ALA	A	347	4.214	6.769	27.114	1.00 32.22
AAAAATOM	2563	N	ASN	A	348	5.968	7.193	25.758	1.00 33.65
AAAAATOM	2564	CA	ASN	A	348	6.681	8.009	26.738	1.00 35.77
AAAAATOM	2565	CB	ASN	A	348	8.078	8.382	26.228	1.00 37.45
AAAAATOM	2566	CG	ASN	A	348	8.996	7.183	26.119	1.00 40.90
AAAAATOM	2567	OD1	ASN	A	348	8.998	6.308	26.989	1.00 43.23
AAAAATOM	2568	ND2	ASN	A	348	9.795	7.140	25.057	1.00 42.50
AAAAATOM	2569	C	ASN	A	348	5.912	9.281	27.074	1.00 35.43
AAAAATOM	2570	O	ASN	A	348	5.824	9.662	28.240	1.00 34.83
AAAAATOM	2571	N	GLU	A	349	5.372	9.943	26.051	1.00 35.34
AAAAATOM	2572	CA	GLU	A	349	4.600	11.164	26.264	1.00 34.80
AAAAATOM	2573	CB	GLU	A	349	4.203	11.802	24.932	1.00 36.04
AAAAATOM	2574	CG	GLU	A	349	5.277	12.681	24.323	1.00 38.86
AAAAATOM	2575	CD	GLU	A	349	5.713	13.801	25.257	1.00 40.72
AAAAATOM	2576	OE1	GLU	A	349	4.836	14.458	25.860	1.00 41.85
AAAAATOM	2577	OE2	GLU	A	349	6.933	14.033	25.385	1.00 42.23
AAAAATOM	2578	C	GLU	A	349	3.357	10.863	27.084	1.00 32.75
AAAAATOM	2579	O	GLU	A	349	2.962	11.658	27.932	1.00 32.53
AAAAATOM	2580	N	VAL	A	350	2.737	9.716	26.827	1.00 31.83
AAAAATOM	2581	CA	VAL	A	350	1.556	9.323	27.583	1.00 31.06
AAAAATOM	2582	CB	VAL	A	350	0.952	8.000	27.049	1.00 31.68
AAAAATOM	2583	CG1	VAL	A	350	0.006	7.406	28.081	1.00 31.12
AAAAATOM	2584	CG2	VAL	A	350	0.205	8.260	25.753	1.00 31.66
AAAAATOM	2585	C	VAL	A	350	1.949	9.135	29.048	1.00 30.82
AAAAATOM	2586	O	VAL	A	350	1.239	9.579	29.953	1.00 30.31
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AAAAATOM	2589	CB	SER	A	351	4.830	7.378	30.610	1.00 31.12
AAAAATOM	2590	OG	SER	A	351	5.292	7.138	31.926	1.00 32.12
AAAAATOM	2591	C	SER	A	351	3.880	9.558	31.351	1.00 30.90
AAAAATOM	2592	O	SER	A	351	3.556	9.731	32.527	1.00 30.97
AAAAATOM	2593	N	ARG	A	352	4.511	10.478	30.633	1.00 31.65
AAAAATOM	2594	CA	ARG	A	352	4.873	11.771	31.193	1.00 33.50
AAAAATOM	2595	CB	ARG	A	352	5.681	12.572	30.172	1.00 35.69
AAAAATOM	2596	CG	ARG	A	352	6.406	13.776	30.753	1.00 40.36
AAAAATOM	2597	CD	ARG	A	352	6.877	14.713	29.652	1.00 43.61
AAAAATOM	2598	NE	ARG	A	352	5.742	15.305	28.947	1.00 47.26
AAAAATOM	2599	CZ	ARG	A	352	5.846	16.181	27.952	1.00 49.17
AAAAATOM	2600	NH1	ARG	A	352	7.043	16.575	27.532	1.00 50.34
AAAAATOM	2601	NH2	ARG	A	352	4.751	16.670	27.381	1.00 49.80
AAAAATOM	2602	C	ARG	A	352	3.623	12.558	31.588	1.00 33.09
AAAAATOM	2603	O	ARG	A	352	3.570	13.159	32.660	1.00 33.61
AAAAATOM	2604	N	VAL	A	353	2.622	12.554	30.713	1.00 32.09
AAAAATOM	2605	CA	VAL	A	353	1.380	13.272	30.975	1.00 32.29
AAAAATOM	2606	CB	VAL	A	353	0.490	13.307	29.714	1.00 31.98
AAAAATOM	2607	CG1	VAL	A	353	-0.897	13.828	30.062	1.00 30.21
AAAAATOM	2608	CG2	VAL	A	353	1.129	14.200	28.665	1.00 30.41
AAAAATOM	2609	C	VAL	A	353	0.596	12.660	32.131	1.00 32.54
AAAAATOM	2610	O	VAL	A	353	0.075	13.379	32.985	1.00 32.79
AAAAATOM	2611	N	ALA	A	354	0.513	11.335	32.159	1.00 32.97
AAAAATOM	2612	CA	ALA	A	354	-0.206	10.650	33.224	1.00 34.65
AAAAATOM	2613	CB	ALA	A	354	-0.157	9.145	33.007	1.00 33.53
AAAAATOM	2614	C	ALA	A	354	0.391	11.002	34.583	1.00 35.84
AAAAATOM	2615	O	ALA	A	354	-0.316	11.026	35.588	1.00 36.31

AAAAATOM	2616	N	ARG	A	355	1.694	11.271	34.609	1.00	38.21
AAAAATOM	2617	CA	ARG	A	355	2.382	11.619	35.852	1.00	41.12
AAAAATOM	2618	CB	ARG	A	355	3.837	11.141	35.802	1.00	42.43
AAAAATOM	2619	CG	ARG	A	355	3.976	9.627	35.701	1.00	44.93
AAAAATOM	2620	CD	ARG	A	355	5.416	9.190	35.457	1.00	47.18
AAAAATOM	2621	NE	ARG	A	355	5.482	7.790	35.042	1.00	48.82
AAAAATOM	2622	CZ	ARG	A	355	5.248	6.754	35.842	1.00	50.06
AAAAATOM	2623	NH1	ARG	A	355	4.939	6.947	37.117	1.00	50.68
AAAAATOM	2624	NH2	ARG	A	355	5.302	5.519	35.360	1.00	50.06
AAAAATOM	2625	C	ARG	A	355	2.333	13.125	36.103	1.00	42.42
AAAAATOM	2626	O	ARG	A	355	2.883	13.621	37.086	1.00	42.30
AAAAATOM	2627	N	ALA	A	356	1.660	13.840	35.203	1.00	43.60
AAAAATOM	2628	CA	ALA	A	356	1.504	15.289	35.294	1.00	44.67
AAAAATOM	2629	CB	ALA	A	356	0.702	15.651	36.547	1.00	45.12
AAAAATOM	2630	C	ALA	A	356	2.830	16.042	35.288	1.00	45.36
AAAAATOM	2631	O	ALA	A	356	2.980	17.042	35.989	1.00	45.40
AAAAATOM	2632	N	LEU	A	357	3.779	15.569	34.487	1.00	46.31
AAAAATOM	2633	CA	LEU	A	357	5.093	16.201	34.392	1.00	47.87
AAAAATOM	2634	CB	LEU	A	357	6.122	15.212	33.843	1.00	47.62
AAAAATOM	2635	CG	LEU	A	357	6.465	14.017	34.734	1.00	47.58
AAAAATOM	2636	CD1	LEU	A	357	7.330	13.041	33.958	1.00	47.32
AAAAATOM	2637	CD2	LEU	A	357	7.187	14.497	35.985	1.00	47.50
AAAAATOM	2638	C	LEU	A	357	5.064	17.438	33.505	1.00	48.87
AAAAATOM	2639	OT1	LEU	A	357	5.458	18.518	33.993	1.00	50.17
AAAAATOM	2640	OT2	LEU	A	357	4.659	17.313	32.330	1.00	50.17
AAAA										
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BBBB										
ATOM	2642	CG	LYS	B	7	-4.666	-44.949	-49.196	1.00	49.02
BBBB										
ATOM	2643	CD	LYS	B	7	-3.162	-44.896	-49.340	1.00	49.96
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ATOM	2644	CE	LYS	B	7	-2.769	-45.054	-50.794	1.00	50.91
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ATOM	2645	NZ	LYS	B	7	-1.300	-45.222	-50.954	1.00	52.39
BBBB										
ATOM	2646	C	LYS	B	7	-6.742	-45.658	-46.035	1.00	43.87
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BBBB										
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BBBB										
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ATOM	2653	CG	ARG	B	8	-8.927	-48.466	-44.677	1.00	43.69
BBBB										
ATOM	2654	CD	ARG	B	8	-9.417	-49.774	-45.269	1.00	46.42
BBBB										
ATOM	2655	NE	ARG	B	8	-10.866	-49.789	-45.425	1.00	50.16
BBBBATOM	2656	CZ	ARG	B	8	-11.722	-49.833	-44.408	1.00	51.89
BBBBATOM	2657	NH1	ARG	B	8	-11.268	-49.869	-43.165	1.00	52.20
BBBBATOM	2658	NH2	ARG	B	8	-13.031	-49.841	-44.631	1.00	53.20
BBBBATOM	2659	C	ARG	B	8	-5.371	-47.512	-43.495	1.00	35.87
BBBBATOM	2660	O	ARG	B	8	-4.474	-48.206	-43.973	1.00	34.76
BBBBATOM	2661	N	LEU	B	9	-5.272	-46.899	-42.321	1.00	32.91
BBBBATOM	2662	CA	LEU	B	9	-4.094	-47.039	-41.477	1.00	30.88
BBBBATOM	2663	CB	LEU	B	9	-3.390	-45.694	-41.278	1.00	30.40
BBBBATOM	2664	CG	LEU	B	9	-2.381	-45.626	-40.119	1.00	29.02
BBBBATOM	2665	CD1	LEU	B	9	-1.157	-46.466	-40.442	1.00	29.47
BBBBATOM	2666	CD2	LEU	B	9	-1.975	-44.178	-39.873	1.00	29.56

BBBBATOM	2667	C	LEU	B	9	-4.513	-47.562	-40.115	1.00 29.67
BBBBATOM	2668	O	LEU	B	9	-5.505	-47.101	-39.543	1.00 28.43
BBBBATOM	2669	N	MET	B	10	-3.772	-48.541	-39.604	1.00 27.75
BBBBATOM	2670	CA	MET	B	10	-4.048	-49.055	-38.275	1.00 26.66
BBBBATOM	2671	CB	MET	B	10	-4.268	-50.571	-38.274	1.00 27.09
BBBBATOM	2672	CG	MET	B	10	-4.496	-51.113	-36.869	1.00 28.55
BBBBATOM	2673	SD	MET	B	10	-5.474	-52.612	-36.799	1.00 29.60
BBBBATOM	2674	CE	MET	B	10	-7.126	-51.913	-36.618	1.00 29.41
BBBBATOM	2675	C	MET	B	10	-2.826	-48.691	-37.448	1.00 25.08
BBBBATOM	2676	O	MET	B	10	-1.690	-48.971	-37.839	1.00 24.38
BBBBATOM	2677	N	VAL	B	11	-3.062	-48.037	-36.317	1.00 23.45
BBBBATOM	2678	CA	VAL	B	11	-1.982	-47.605	-35.449	1.00 23.16
BBBBATOM	2679	CB	VAL	B	11	-2.159	-46.116	-35.029	1.00 23.01
BBBBATOM	2680	CG1	VAL	B	11	-0.971	-45.666	-34.184	1.00 20.91
BBBBATOM	2681	CG2	VAL	B	11	-2.305	-45.225	-36.276	1.00 23.82
BBBBATOM	2682	C	VAL	B	11	-1.935	-48.461	-34.184	1.00 23.59
BBBBATOM	2683	O	VAL	B	11	-2.962	-48.712	-33.567	1.00 23.24
BBBBATOM	2684	N	MET	B	12	-0.734	-48.902	-33.817	1.00 23.68
BBBBATOM	2685	CA	MET	B	12	-0.523	-49.707	-32.613	1.00 24.54
BBBBATOM	2686	CB	MET	B	12	0.192	-51.019	-32.971	1.00 24.28
BBBBATOM	2687	CG	MET	B	12	-0.402	-51.726	-34.188	1.00 25.19
BBBBATOM	2688	SD	MET	B	12	0.399	-53.284	-34.669	1.00 26.54
BBBBATOM	2689	CE	MET	B	12	1.990	-52.691	-35.289	1.00 22.99
BBBBATOM	2690	C	MET	B	12	0.361	-48.840	-31.720	1.00 25.31
BBBBATOM	2691	O	MET	B	12	1.546	-48.645	-32.006	1.00 23.88
BBBBATOM	2692	N	ALA	B	13	-0.224	-48.292	-30.657	1.00 27.08
BBBBATOM	2693	CA	ALA	B	13	0.508	-47.410	-29.752	1.00 29.43
BBBBATOM	2694	CB	ALA	B	13	0.747	-46.074	-30.429	1.00 28.82
BBBBATOM	2695	C	ALA	B	13	-0.239	-47.192	-28.436	1.00 31.80
BBBBATOM	2696	O	ALA	B	13	-1.143	-46.350	-28.352	1.00 32.16
BBBBATOM	2697	N	GLY	B	14	0.150	-47.934	-27.405	1.00 32.46
BBBBATOM	2698	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00 33.82
BBBBATOM	2699	C	GLY	B	14	-0.107	-46.595	-25.299	1.00 34.82
BBBBATOM	2700	O	GLY	B	14	0.975	-46.040	-25.479	1.00 35.47
BBBBATOM	2701	N	GLY	B	15	-0.986	-46.188	-24.385	1.00 35.56
BBBBATOM	2702	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00 36.08
BBBBATOM	2703	C	GLY	B	15	0.539	-45.254	-22.683	1.00 36.84
BBBBATOM	2704	O	GLY	B	15	1.293	-44.311	-22.426	1.00 36.03
BBBBATOM	2705	N	THR	B	16	0.755	-46.488	-22.240	1.00 36.65
BBBBATOM	2706	CA	THR	B	16	1.920	-46.787	-21.421	1.00 38.51
BBBBATOM	2707	CB	THR	B	16	1.926	-48.258	-20.974	1.00 38.51
BBBBATOM	2708	OG1	THR	B	16	0.686	-48.558	-20.321	1.00 38.39
BBBBATOM	2709	CG2	THR	B	16	3.075	-48.518	-20.005	1.00 39.11
BBBBATOM	2710	C	THR	B	16	3.158	-46.497	-22.264	1.00 38.35
BBBBATOM	2711	O	THR	B	16	3.191	-46.798	-23.460	1.00 39.90
BBBBATOM	2712	N	GLY	B	17	4.168	-45.897	-21.649	1.00 37.68
BBBBATOM	2713	CA	GLY	B	17	5.367	-45.567	-22.392	1.00 36.57
BBBBATOM	2714	C	GLY	B	17	5.161	-44.303	-23.211	1.00 35.56
BBBBATOM	2715	O	GLY	B	17	6.079	-43.843	-23.890	1.00 35.03
BBBBATOM	2716	N	GLY	B	18	3.949	-43.752	-23.150	1.00 33.83
BBBBATOM	2717	CA	GLY	B	18	3.631	-42.529	-23.872	1.00 33.48
BBBBATOM	2718	C	GLY	B	18	3.825	-42.593	-25.378	1.00 33.12
BBBBATOM	2719	O	GLY	B	18	4.345	-41.650	-25.984	1.00 35.38
BBBBATOM	2720	N	HIS	B	19	3.416	-43.699	-25.988	1.00 30.26
BBBBATOM	2721	CA	HIS	B	19	3.548	-43.865	-27.435	1.00 28.22
BBBBATOM	2722	CB	HIS	B	19	3.772	-45.349	-27.779	1.00 25.81
BBBBATOM	2723	CG	HIS	B	19	4.957	-45.966	-27.094	1.00 25.35
BBBBATOM	2724	CD2	HIS	B	19	6.281	-45.694	-27.184	1.00 24.18
BBBBATOM	2725	ND1	HIS	B	19	4.845	-47.025	-26.217	1.00 24.57
BBBBATOM	2726	CE1	HIS	B	19	6.046	-47.380	-25.798	1.00 23.08
BBBBATOM	2727	NE2	HIS	B	19	6.936	-46.589	-26.369	1.00 25.51
BBBBATOM	2728	C	HIS	B	19	2.280	-43.370	-28.144	1.00 27.91
BBBBATOM	2729	O	HIS	B	19	2.300	-43.049	-29.337	1.00 26.91
BBBBATOM	2730	N	VAL	B	20	1.180	-43.310	-27.402	1.00 27.65
BBBBATOM	2731	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00 27.77
BBBBATOM	2732	CB	VAL	B	20	-1.248	-43.080	-26.942	1.00 28.57

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BBBBATOM	2733	CG1	VAL	B	20	-1.082	-42.114	-25.787	1.00 30.03
BBBBATOM	2734	CG2	VAL	B	20	-2.602	-42.873	-27.631	1.00 26.82
BBBBATOM	2735	C	VAL	B	20	-0.140	-41.452	-28.470	1.00 27.57
BBBBATOM	2736	O	VAL	B	20	-0.771	-41.172	-29.486	1.00 27.12
BBBBATOM	2737	N	PHE	B	21	0.528	-40.543	-27.770	1.00 28.03
BBBBATOM	2738	CA	PHE	B	21	0.517	-39.136	-28.160	1.00 29.00
BBBBATOM	2739	CB	PHE	B	21	1.215	-38.289	-27.094	1.00 30.27
BBBBATOM	2740	CG	PHE	B	21	0.565	-38.383	-25.746	1.00 33.59
BBBBATOM	2741	CD1	PHE	B	21	-0.764	-37.999	-25.578	1.00 33.84
BBBBATOM	2742	CD2	PHE	B	21	1.256	-38.909	-24.659	1.00 35.22
BBBBATOM	2743	CE1	PHE	B	21	-1.397	-38.142	-24.350	1.00 35.17
BBBBATOM	2744	CE2	PHE	B	21	0.630	-39.057	-23.422	1.00 36.08
BBBBATOM	2745	CZ	PHE	B	21	-0.700	-38.673	-23.269	1.00 35.65
BBBBATOM	2746	C	PHE	B	21	1.129	-38.898	-29.535	1.00 28.53
BBBBATOM	2747	O	PHE	B	21	0.521	-38.236	-30.378	1.00 28.69
BBBBATOM	2748	N	PRO	B	22	2.336	-39.430	-29.781	1.00 27.41
BBBBATOM	2749	CD	PRO	B	22	3.251	-40.074	-28.819	1.00 27.82
BBBBATOM	2750	CA	PRO	B	22	2.986	-39.252	-31.086	1.00 26.12
BBBBATOM	2751	CB	PRO	B	22	4.362	-39.884	-30.883	1.00 27.48
BBBBATOM	2752	CG	PRO	B	22	4.594	-39.757	-29.403	1.00 28.99
BBBBATOM	2753	C	PRO	B	22	2.188	-39.972	-32.176	1.00 26.37
BBBBATOM	2754	O	PRO	B	22	2.129	-39.522	-33.321	1.00 24.40
BBBBATOM	2755	N	GLY	B	23	1.585	-41.102	-31.807	1.00 24.71
BBBBATOM	2756	CA	GLY	B	23	0.787	-41.864	-32.752	1.00 25.07
BBBBATOM	2757	C	GLY	B	23	-0.459	-41.088	-33.144	1.00 25.00
BBBBATOM	2758	O	GLY	B	23	-0.913	-41.144	-34.295	1.00 23.40
BBBBATOM	2759	N	LEU	B	24	-1.014	-40.366	-32.176	1.00 24.65
BBBBATOM	2760	CA	LEU	B	24	-2.201	-39.551	-32.401	1.00 25.32
BBBBATOM	2761	CB	LEU	B	24	-2.732	-39.017	-31.064	1.00 25.08
BBBBATOM	2762	CG	LEU	B	24	-3.594	-39.997	-30.264	1.00 23.58
BBBBATOM	2763	CD1	LEU	B	24	-3.823	-39.482	-28.828	1.00 25.41
BBBBATOM	2764	CD2	LEU	B	24	-4.919	-40.192	-30.998	1.00 24.78
BBBBATOM	2765	C	LEU	B	24	-1.843	-38.397	-33.336	1.00 25.69
BBBBATOM	2766	O	LEU	B	24	-2.634	-38.017	-34.204	1.00 25.99
BBBBATOM	2767	N	ALA	B	25	-0.644	-37.850	-33.164	1.00 24.89
BBBBATOM	2768	CA	ALA	B	25	-0.197	-36.754	-34.013	1.00 25.94
BBBBATOM	2769	CB	ALA	B	25	1.195	-36.278	-33.590	1.00 25.12
BBBBATOM	2770	C	ALA	B	25	-0.171	-37.207	-35.469	1.00 27.14
BBBBATOM	2771	O	ALA	B	25	-0.626	-36.483	-36.354	1.00 27.46
BBBBATOM	2772	N	VAL	B	26	0.368	-38.403	-35.709	1.00 26.50
BBBBATOM	2773	CA	VAL	B	26	0.466	-38.955	-37.056	1.00 25.70
BBBBATOM	2774	CB	VAL	B	26	1.373	-40.226	-37.081	1.00 26.22
BBBBATOM	2775	CG1	VAL	B	26	1.410	-40.833	-38.479	1.00 26.25
BBBBATOM	2776	CG2	VAL	B	26	2.778	-39.861	-36.631	1.00 24.56
BBBBATOM	2777	C	VAL	B	26	-0.908	-39.310	-37.612	1.00 26.20
BBBBATOM	2778	O	VAL	B	26	-1.178	-39.091	-38.796	1.00 25.87
BBBBATOM	2779	N	ALA	B	27	-1.777	-39.851	-36.764	1.00 24.68
BBBBATOM	2780	CA	ALA	B	27	-3.116	-40.222	-37.199	1.00 26.15
BBBBATOM	2781	CB	ALA	B	27	-3.868	-40.909	-36.066	1.00 26.23
BBBBATOM	2782	C	ALA	B	27	-3.888	-38.984	-37.661	1.00 27.60
BBBBATOM	2783	O	ALA	B	27	-4.492	-38.985	-38.736	1.00 27.05
BBBBATOM	2784	N	HIS	B	28	-3.864	-37.933	-36.847	1.00 27.68
BBBBATOM	2785	CA	HIS	B	28	-4.574	-36.702	-37.190	1.00 29.32
BBBBATOM	2786	CB	HIS	B	28	-4.498	-35.693	-36.039	1.00 27.05
BBBBATOM	2787	CG	HIS	B	28	-5.491	-35.957	-34.952	1.00 27.65
BBBBATOM	2788	CD2	HIS	B	28	-5.327	-36.213	-33.632	1.00 26.92
BBBBATOM	2789	ND1	HIS	B	28	-6.850	-36.010	-35.188	1.00 27.29
BBBBATOM	2790	CE1	HIS	B	28	-7.479	-36.290	-34.060	1.00 26.85
BBBBATOM	2791	NE2	HIS	B	28	-6.578	-36.417	-33.101	1.00 27.78
BBBBATOM	2792	C	HIS	B	28	-4.018	-36.095	-38.462	1.00 30.24
BBBBATOM	2793	O	HIS	B	28	-4.766	-35.589	-39.297	1.00 31.14
BBBBATOM	2794	N	HIS	B	29	-2.702	-36.164	-38.618	1.00 31.42
BBBBATOM	2795	CA	HIS	B	29	-2.070	-35.623	-39.806	1.00 32.38
BBBBATOM	2796	CB	HIS	B	29	-0.554	-35.764	-39.720	1.00 33.49
BBBBATOM	2797	CG	HIS	B	29	0.177	-34.957	-40.743	1.00 35.61
BBBBATOM	2798	CD2	HIS	B	29	0.667	-35.292	-41.960	1.00 36.38

BBBBATOM	2799	ND1	HIS	B	29	0.436	-33.612	-40.583	1.00 37.53
BBBBATOM	2800	CE1	HIS	B	29	1.055	-33.155	-41.657	1.00 37.93
BBBBATOM	2801	NE2	HIS	B	29	1.207	-34.154	-42.508	1.00 37.24
BBBBATOM	2802	C	HIS	B	29	-2.567	-36.324	-41.068	1.00 33.00
BBBBATOM	2803	O	HIS	B	29	-2.845	-35.674	-42.078	1.00 33.02
BBBBATOM	2804	N	LEU	B	30	-2.676	-37.650	-41.012	1.00 31.69
BBBBATOM	2805	CA	LEU	B	30	-3.136	-38.417	-42.162	1.00 32.00
BBBBATOM	2806	CB	LEU	B	30	-2.701	-39.883	-42.033	1.00 30.44
BBBBATOM	2807	CG	LEU	B	30	-1.191	-40.099	-42.203	1.00 29.95
BBBBATOM	2808	CD1	LEU	B	30	-0.823	-41.550	-41.898	1.00 28.64
BBBBATOM	2809	CD2	LEU	B	30	-0.785	-39.736	-43.621	1.00 28.97
BBBBATOM	2810	C	LEU	B	30	-4.641	-38.332	-42.375	1.00 32.37
BBBBATOM	2811	O	LEU	B	30	-5.109	-38.414	-43.507	1.00 33.16
BBBBATOM	2812	N	MET	B	31	-5.401	-38.168	-41.297	1.00 33.50
BBBBATOM	2813	CA	MET	B	31	-6.849	-38.064	-41.424	1.00 34.91
BBBBATOM	2814	CB	MET	B	31	-7.514	-38.061	-40.048	1.00 35.67
BBBBATOM	2815	CG	MET	B	31	-7.536	-39.424	-39.391	1.00 36.44
BBBBATOM	2816	SD	MET	B	31	-8.407	-39.436	-37.827	1.00 37.84
BBBBATOM	2817	CE	MET	B	31	-7.095	-39.039	-36.719	1.00 37.80
BBBBATOM	2818	C	MET	B	31	-7.197	-36.786	-42.173	1.00 35.99
BBBBATOM	2819	O	MET	B	31	-8.224	-36.710	-42.847	1.00 37.36
BBBBATOM	2820	N	ALA	B	32	-6.326	-35.791	-42.052	1.00 36.39
BBBBATOM	2821	CA	ALA	B	32	-6.510	-34.511	-42.722	1.00 37.55
BBBBATOM	2822	CB	ALA	B	32	-5.622	-33.458	-42.073	1.00 36.85
BBBBATOM	2823	C	ALA	B	32	-6.151	-34.663	-44.205	1.00 38.60
BBBBATOM	2824	O	ALA	B	32	-6.392	-33.760	-45.013	1.00 38.04
BBBBATOM	2825	N	GLN	B	33	-5.569	-35.809	-44.555	1.00 38.35
BBBBATOM	2826	CA	GLN	B	33	-5.182	-36.070	-45.938	1.00 38.24
BBBBATOM	2827	CB	GLN	B	33	-3.792	-36.706	-46.011	1.00 39.81
BBBBATOM	2828	CG	GLN	B	33	-2.771	-36.162	-45.028	1.00 41.67
BBBBATOM	2829	CD	GLN	B	33	-2.269	-34.781	-45.384	1.00 41.96
BBBBATOM	2830	OE1	GLN	B	33	-1.735	-34.559	-46.471	1.00 41.35
BBBBATOM	2831	NE2	GLN	B	33	-2.423	-33.843	-44.456	1.00 42.42
BBBBATOM	2832	C	GLN	B	33	-6.187	-37.027	-46.556	1.00 36.70
BBBBATOM	2833	O	GLN	B	33	-5.970	-37.541	-47.647	1.00 36.47
BBBBATOM	2834	N	GLY	B	34	-7.281	-37.274	-45.845	1.00 36.09
BBBBATOM	2835	CA	GLY	B	34	-8.305	-38.169	-46.353	1.00 35.75
BBBBATOM	2836	C	GLY	B	34	-8.219	-39.600	-45.837	1.00 35.33
BBBBATOM	2837	O	GLY	B	34	-9.075	-40.426	-46.146	1.00 34.43
BBBBATOM	2838	N	TRP	B	35	-7.196	-39.896	-45.042	1.00 35.23
BBBBATOM	2839	CA	TRP	B	35	-7.016	-41.246	-44.508	1.00 34.58
BBBBATOM	2840	CB	TRP	B	35	-5.618	-41.400	-43.908	1.00 35.03
BBBBATOM	2841	CG	TRP	B	35	-4.511	-41.558	-44.901	1.00 34.87
BBBBATOM	2842	CD2	TRP	B	35	-3.666	-42.704	-45.060	1.00 35.81
BBBBATOM	2843	CE2	TRP	B	35	-2.733	-42.399	-46.076	1.00 35.60
BBBBATOM	2844	CE3	TRP	B	35	-3.605	-43.961	-44.441	1.00 36.59
BBBBATOM	2845	CD1	TRP	B	35	-4.075	-40.633	-45.803	1.00 35.62
BBBBATOM	2846	NE1	TRP	B	35	-3.004	-41.129	-46.513	1.00 34.95
BBBBATOM	2847	CZ2	TRP	B	35	-1.746	-43.305	-46.488	1.00 37.19
BBBBATOM	2848	CZ3	TRP	B	35	-2.620	-44.865	-44.852	1.00 36.85
BBBBATOM	2849	CH2	TRP	B	35	-1.705	-44.528	-45.867	1.00 36.87
BBBBATOM	2850	C	TRP	B	35	-8.022	-41.670	-43.449	1.00 34.58
BBBBATOM	2851	O	TRP	B	35	-8.546	-40.850	-42.699	1.00 33.58
BBBBATOM	2852	N	GLN	B	36	-8.295	-42.969	-43.410	1.00 34.54
BBBBATOM	2853	CA	GLN	B	36	-9.175	-43.535	-42.402	1.00 35.40
BBBBATOM	2854	CB	GLN	B	36	-10.095	-44.596	-43.003	1.00 37.42
BBBBATOM	2855	CG	GLN	B	36	-11.219	-44.027	-43.862	1.00 41.66
BBBBATOM	2856	CD	GLN	B	36	-11.996	-45.103	-44.601	1.00 44.12
BBBBATOM	2857	OE1	GLN	B	36	-12.988	-44.816	-45.277	1.00 45.76
BBBBATOM	2858	NE2	GLN	B	36	-11.546	-46.350	-44.480	1.00 44.99
BBBBATOM	2859	C	GLN	B	36	-8.183	-44.186	-41.451	1.00 34.89
BBBBATOM	2860	O	GLN	B	36	-7.272	-44.885	-41.889	1.00 34.58
BBBBATOM	2861	N	VAL	B	37	-8.336	-43.941	-40.158	1.00 35.26
BBBBATOM	2862	CA	VAL	B	37	-7.417	-44.516	-39.184	1.00 34.16
BBBBATOM	2863	CB	VAL	B	37	-6.561	-43.417	-38.509	1.00 34.99
BBBBATOM	2864	CG1	VAL	B	37	-5.630	-44.032	-37.479	1.00 34.72

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BBBBATOM	2865	CG2	VAL	B	37	-5.755	-42.668	-39.552	1.00 34.06
BBBBATOM	2866	C	VAL	B	37	-8.166	-45.288	-38.109	1.00 34.02
BBBBATOM	2867	O	VAL	B	37	-9.207	-44.849	-37.618	1.00 33.01
BBBBATOM	2868	N	ARG	B	38	-7.629	-46.451	-37.758	1.00 32.20
BBBBATOM	2869	CA	ARG	B	38	-8.219	-47.286	-36.730	1.00 31.56
BBBBATOM	2870	CB	ARG	B	38	-8.811	-48.554	-37.344	1.00 33.53
BBBBATOM	2871	CG	ARG	B	38	-9.706	-49.324	-36.397	1.00 36.77
BBBBATOM	2872	CD	ARG	B	38	-11.107	-49.511	-36.975	1.00 38.80
BBBBATOM	2873	NE	ARG	B	38	-12.000	-50.108	-35.989	1.00 41.24
BBBBATOM	2874	CZ	ARG	B	38	-13.304	-50.293	-36.161	1.00 43.18
BBBBATOM	2875	NH1	ARG	B	38	-13.892	-49.927	-37.294	1.00 43.21
BBBBATOM	2876	NH2	ARG	B	38	-14.026	-50.839	-35.189	1.00 44.37
BBBBATOM	2877	C	ARG	B	38	-7.097	-47.628	-35.751	1.00 30.48
BBBBATOM	2878	O	ARG	B	38	-5.936	-47.742	-36.134	1.00 29.62
BBBBATOM	2879	N	TRP	B	39	-7.447	-47.782	-34.484	1.00 28.40
BBBBATOM	2880	CA	TRP	B	39	-6.456	-48.070	-33.471	1.00 27.41
BBBBATOM	2881	CB	TRP	B	39	-6.696	-47.145	-32.291	1.00 27.98
BBBBATOM	2882	CG	TRP	B	39	-5.480	-46.788	-31.568	1.00 28.00
BBBBATOM	2883	CD2	TRP	B	39	-4.677	-45.627	-31.784	1.00 28.42
BBBBATOM	2884	CE2	TRP	B	39	-3.625	-45.673	-30.851	1.00 28.85
BBBBATOM	2885	CE3	TRP	B	39	-4.749	-44.549	-32.680	1.00 29.78
BBBBATOM	2886	CD1	TRP	B	39	-4.898	-47.476	-30.549	1.00 28.26
BBBBATOM	2887	NE1	TRP	B	39	-3.783	-46.812	-30.111	1.00 28.48
BBBBATOM	2888	CZ2	TRP	B	39	-2.648	-44.684	-30.778	1.00 30.55
BBBBATOM	2889	CZ3	TRP	B	39	-3.770	-43.561	-32.610	1.00 29.22
BBBBATOM	2890	CH2	TRP	B	39	-2.734	-43.639	-31.662	1.00 30.90
BBBBATOM	2891	C	TRP	B	39	-6.478	-49.517	-32.999	1.00 25.82
BBBBATOM	2892	O	TRP	B	39	-7.509	-50.176	-33.055	1.00 24.87
BBBBATOM	2893	N	LEU	B	40	-5.323	-50.004	-32.549	1.00 25.21
BBBBATOM	2894	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00 24.71
BBBBATOM	2895	CB	LEU	B	40	-4.326	-52.221	-32.952	1.00 25.21
BBBBATOM	2896	CG	LEU	B	40	-4.416	-53.754	-32.868	1.00 26.95
BBBBATOM	2897	CD1	LEU	B	40	-3.037	-54.334	-32.571	1.00 27.63
BBBBATOM	2898	CD2	LEU	B	40	-5.421	-54.179	-31.817	1.00 26.69
BBBBATOM	2899	C	LEU	B	40	-4.535	-51.235	-30.655	1.00 23.33
BBBBATOM	2900	O	LEU	B	40	-3.387	-50.824	-30.563	1.00 23.43
BBBBATOM	2901	N	GLY	B	41	-5.260	-51.567	-29.591	1.00 24.01
BBBBATOM	2902	CA	GLY	B	41	-4.691	-51.450	-28.257	1.00 23.47
BBBBATOM	2903	C	GLY	B	41	-5.292	-52.479	-27.322	1.00 23.99
BBBBATOM	2904	O	GLY	B	41	-5.797	-53.498	-27.785	1.00 22.90
BBBBATOM	2905	N	THR	B	42	-5.225	-52.225	-26.017	1.00 26.62
BBBBATOM	2906	CA	THR	B	42	-5.787	-53.141	-25.027	1.00 29.84
BBBBATOM	2907	CB	THR	B	42	-4.693	-53.715	-24.092	1.00 30.17
BBBBATOM	2908	OG1	THR	B	42	-4.019	-52.647	-23.418	1.00 30.77
BBBBATOM	2909	CG2	THR	B	42	-3.683	-54.514	-24.900	1.00 31.30
BBBBATOM	2910	C	THR	B	42	-6.852	-52.420	-24.200	1.00 32.04
BBBBATOM	2911	O	THR	B	42	-6.737	-51.226	-23.924	1.00 31.27
BBBBATOM	2912	N	ALA	B	43	-7.881	-53.160	-23.801	1.00 35.37
BBBBATOM	2913	CA	ALA	B	43	-9.000	-52.595	-23.047	1.00 38.81
BBBBATOM	2914	CB	ALA	B	43	-10.063	-53.669	-22.835	1.00 38.49
BBBBATOM	2915	C	ALA	B	43	-8.671	-51.928	-21.713	1.00 41.06
BBBBATOM	2916	O	ALA	B	43	-9.224	-50.875	-21.391	1.00 42.22
BBBBATOM	2917	N	ASP	B	44	-7.777	-52.521	-20.931	1.00 43.18
BBBBATOM	2918	CA	ASP	B	44	-7.455	-51.942	-19.632	1.00 44.47
BBBBATOM	2919	CB	ASP	B	44	-7.311	-53.057	-18.586	1.00 46.93
BBBBATOM	2920	CG	ASP	B	44	-8.646	-53.724	-18.255	1.00 48.65
BBBBATOM	2921	OD1	ASP	B	44	-9.553	-53.026	-17.753	1.00 50.52
BBBBATOM	2922	OD2	ASP	B	44	-8.791	-54.943	-18.498	1.00 49.40
BBBBATOM	2923	C	ASP	B	44	-6.236	-51.025	-19.598	1.00 44.13
BBBBATOM	2924	O	ASP	B	44	-5.520	-50.968	-18.595	1.00 45.05
BBBBATOM	2925	N	ARG	B	45	-6.001	-50.307	-20.692	1.00 42.34
BBBBATOM	2926	CA	ARG	B	45	-4.887	-49.367	-20.763	1.00 40.44
BBBBATOM	2927	CB	ARG	B	45	-3.802	-49.869	-21.725	1.00 41.87
BBBBATOM	2928	CG	ARG	B	45	-2.935	-50.994	-21.149	1.00 43.86
BBBBATOM	2929	CD	ARG	B	45	-2.218	-50.541	-19.881	1.00 45.24
BBBBATOM	2930	NE	ARG	B	45	-1.385	-51.582	-19.277	1.00 46.96

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BBBBATOM   2931  CZ   ARG B  45    -1.840 -52.753 -18.839  1.00 47.69
BBBBATOM   2932  NH1  ARG B  45    -3.130 -53.051 -18.937  1.00 48.59
BBBBATOM   2933  NH2  ARG B  45    -1.005 -53.626 -18.289  1.00 48.33
BBBBATOM   2934  C    ARG B  45    -5.390 -47.992 -21.195  1.00 38.74
BBBBATOM   2935  O    ARG B  45    -6.486 -47.866 -21.738  1.00 37.69
BBBBATOM   2936  N    MET B  46    -4.567 -46.977 -20.955  1.00 37.09
BBBBATOM   2937  CA   MET B  46    -4.881 -45.581 -21.249  1.00 36.33
BBBBATOM   2938  CB   MET B  46    -3.644 -44.725 -20.945  1.00 37.92
BBBBATOM   2939  CG   MET B  46    -3.873 -43.222 -20.952  1.00 40.65
BBBBATOM   2940  SD   MET B  46    -3.420 -42.436 -22.517  1.00 44.22
BBBBATOM   2941  CE   MET B  46    -1.720 -41.959 -22.168  1.00 41.80
BBBBATOM   2942  C    MET B  46    -5.430 -45.239 -22.643  1.00 34.96
BBBBATOM   2943  O    MET B  46    -6.264 -44.338 -22.774  1.00 33.21
BBBBATOM   2944  N    GLU B  47    -4.976 -45.941 -23.678  1.00 32.85
BBBBATOM   2945  CA   GLU B  47    -5.458 -45.655 -25.029  1.00 31.79
BBBBATOM   2946  CB   GLU B  47    -4.624 -46.402 -26.080  1.00 30.62
BBBBATOM   2947  CG   GLU B  47    -4.755 -47.922 -26.051  1.00 29.85
BBBBATOM   2948  CD   GLU B  47    -3.793 -48.597 -25.082  1.00 29.78
BBBBATOM   2949  OE1  GLU B  47    -3.188 -47.895 -24.247  1.00 28.76
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BBBBATOM   2951  C    GLU B  47    -6.938 -46.017 -25.191  1.00 31.81
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BBBBATOM   2953  N    ALA B  48    -7.428 -46.924 -24.352  1.00 31.55
BBBBATOM   2954  CA   ALA B  48    -8.821 -47.344 -24.414  1.00 32.58
BBBBATOM   2955  CB   ALA B  48    -9.085 -48.450 -23.384  1.00 33.19
BBBBATOM   2956  C    ALA B  48    -9.761 -46.168 -24.164  1.00 33.37
BBBBATOM   2957  O    ALA B  48   -10.860 -46.114 -24.716  1.00 33.81
BBBBATOM   2958  N    ASP B  49    -9.328 -45.232 -23.328  1.00 34.05
BBBBATOM   2959  CA   ASP B  49   -10.143 -44.065 -23.009  1.00 35.60
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BBBBATOM   2961  CG   ASP B  49   -10.645 -44.812 -20.628  1.00 39.54
BBBBATOM   2962  OD1  ASP B  49   -11.835 -45.144 -20.825  1.00 40.82
BBBBATOM   2963  OD2  ASP B  49    -9.939 -45.323 -19.730  1.00 39.49
BBBBATOM   2964  C    ASP B  49    -9.768 -42.832 -23.831  1.00 34.79
BBBBATOM   2965  O    ASP B  49   -10.637 -42.064 -24.241  1.00 35.85
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BBBBATOM   2967  CA   LEU B  50    -8.026 -41.484 -24.840  1.00 33.49
BBBBATOM   2968  CB   LEU B  50    -6.526 -41.264 -24.635  1.00 33.25
BBBBATOM   2969  CG   LEU B  50    -6.001 -39.986 -25.299  1.00 33.36
BBBBATOM   2970  CD1  LEU B  50    -6.679 -38.771 -24.659  1.00 34.04
BBBBATOM   2971  CD2  LEU B  50    -4.496 -39.894 -25.157  1.00 33.08
BBBBATOM   2972  C    LEU B  50    -8.320 -41.486 -26.337  1.00 33.52
BBBBATOM   2973  O    LEU B  50    -8.769 -40.477 -26.882  1.00 32.52
BBBBATOM   2974  N    VAL B  51    -8.073 -42.605 -27.011  1.00 32.94
BBBBATOM   2975  CA   VAL B  51    -8.299 -42.641 -28.449  1.00 32.68
BBBBATOM   2976  CB   VAL B  51    -7.829 -43.982 -29.058  1.00 33.06
BBBBATOM   2977  CG1  VAL B  51    -8.115 -44.013 -30.565  1.00 31.54
BBBBATOM   2978  CG2  VAL B  51    -6.329 -44.145 -28.813  1.00 31.45
BBBBATOM   2979  C    VAL B  51    -9.747 -42.348 -28.829  1.00 33.08
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BBBBATOM   2981  N    PRO B  52   -10.721 -42.900 -28.085  1.00 33.67
BBBBATOM   2982  CD   PRO B  52   -10.667 -44.012 -27.119  1.00 33.29
BBBBATOM   2983  CA   PRO B  52   -12.111 -42.601 -28.453  1.00 34.43
BBBBATOM   2984  CB   PRO B  52   -12.915 -43.465 -27.489  1.00 34.36
BBBBATOM   2985  CG   PRO B  52   -12.021 -44.661 -27.307  1.00 33.77
BBBBATOM   2986  C    PRO B  52   -12.422 -41.111 -28.294  1.00 35.67
BBBBATOM   2987  O    PRO B  52   -13.219 -40.548 -29.048  1.00 36.65
BBBBATOM   2988  N    LYS B  53   -11.790 -40.478 -27.310  1.00 35.75
BBBBATOM   2989  CA   LYS B  53   -11.998 -39.054 -27.064  1.00 36.73
BBBBATOM   2990  CB   LYS B  53   -11.334 -38.633 -25.746  1.00 37.14
BBBBATOM   2991  CG   LYS B  53   -12.020 -39.207 -24.514  1.00 38.38
BBBBATOM   2992  CD   LYS B  53   -11.368 -38.746 -23.218  1.00 39.34
BBBBATOM   2993  CE   LYS B  53   -12.057 -39.379 -22.012  1.00 40.74
BBBBATOM   2994  NZ   LYS B  53   -11.352 -39.092 -20.725  1.00 40.94
BBBBATOM   2995  C    LYS B  53   -11.445 -38.231 -28.220  1.00 36.11
BBBBATOM   2996  O    LYS B  53   -11.703 -37.036 -28.323  1.00 36.71
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BBBBATOM	2997	N	HIS	B	54	-10.688	-38.881	-29.096	1.00	35.60
BBBBATOM	2998	CA	HIS	B	54	-10.116	-38.212	-30.259	1.00	34.62
BBBBATOM	2999	CB	HIS	B	54	-8.666	-38.647	-30.464	1.00	34.78
BBBBATOM	3000	CG	HIS	B	54	-7.676	-37.810	-29.721	1.00	33.79
BBBBATOM	3001	CD2	HIS	B	54	-7.360	-37.760	-28.406	1.00	33.76
BBBBATOM	3002	ND1	HIS	B	54	-6.884	-36.869	-30.343	1.00	34.27
BBBBATOM	3003	CE1	HIS	B	54	-6.120	-36.277	-29.441	1.00	34.41
BBBBATOM	3004	NE2	HIS	B	54	-6.390	-36.799	-28.258	1.00	33.91
BBBBATOM	3005	C	HIS	B	54	-10.919	-38.524	-31.512	1.00	34.28
BBBBATOM	3006	O	HIS	B	54	-10.487	-38.224	-32.620	1.00	34.99
BBBBATOM	3007	N	GLY	B	55	-12.082	-39.140	-31.325	1.00	34.47
BBBBATOM	3008	CA	GLY	B	55	-12.938	-39.481	-32.447	1.00	35.34
BBBBATOM	3009	C	GLY	B	55	-12.427	-40.619	-33.310	1.00	36.18
BBBBATOM	3010	O	GLY	B	55	-12.883	-40.799	-34.442	1.00	35.99
BBBBATOM	3011	N	ILE	B	56	-11.490	-41.399	-32.776	1.00	35.32
BBBBATOM	3012	CA	ILE	B	56	-10.909	-42.517	-33.514	1.00	33.81
BBBBATOM	3013	CB	ILE	B	56	-9.374	-42.445	-33.462	1.00	33.36
BBBBATOM	3014	CG2	ILE	B	56	-8.761	-43.602	-34.245	1.00	32.87
BBBBATOM	3015	CG1	ILE	B	56	-8.916	-41.097	-34.029	1.00	32.05
BBBBATOM	3016	CD1	ILE	B	56	-7.461	-40.792	-33.818	1.00	30.35
BBBBATOM	3017	C	ILE	B	56	-11.375	-43.859	-32.956	1.00	34.45
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BBBBATOM	3019	N	GLU	B	57	-11.764	-44.758	-33.855	1.00	33.40
BBBBATOM	3020	CA	GLU	B	57	-12.228	-46.083	-33.467	1.00	34.16
BBBBATOM	3021	CB	GLU	B	57	-12.905	-46.769	-34.651	1.00	37.41
BBBBATOM	3022	CG	GLU	B	57	-14.064	-45.982	-35.244	1.00	42.10
BBBBATOM	3023	CD	GLU	B	57	-14.653	-46.659	-36.465	1.00	45.50
BBBBATOM	3024	OE1	GLU	B	57	-13.903	-46.875	-37.448	1.00	46.39
BBBBATOM	3025	OE2	GLU	B	57	-15.866	-46.977	-36.441	1.00	48.36
BBBBATOM	3026	C	GLU	B	57	-11.044	-46.923	-33.005	1.00	33.01
BBBBATOM	3027	O	GLU	B	57	-9.931	-46.769	-33.504	1.00	31.58
BBBBATOM	3028	N	ILE	B	58	-11.287	-47.817	-32.056	1.00	31.85
BBBBATOM	3029	CA	ILE	B	58	-10.217	-48.658	-31.553	1.00	31.38
BBBBATOM	3030	CB	ILE	B	58	-9.651	-48.099	-30.223	1.00	30.95
BBBBATOM	3031	CG2	ILE	B	58	-10.769	-47.946	-29.205	1.00	31.48
BBBBATOM	3032	CG1	ILE	B	58	-8.553	-49.030	-29.690	1.00	31.13
BBBBATOM	3033	CD1	ILE	B	58	-7.736	-48.437	-28.572	1.00	29.87
BBBBATOM	3034	C	ILE	B	58	-10.647	-50.102	-31.357	1.00	31.67
BBBBATOM	3035	O	ILE	B	58	-11.716	-50.384	-30.801	1.00	30.68
BBBBATOM	3036	N	ASP	B	59	-9.807	-51.011	-31.844	1.00	30.76
BBBBATOM	3037	CA	ASP	B	59	-10.039	-52.442	-31.720	1.00	31.09
BBBBATOM	3038	CB	ASP	B	59	-9.732	-53.153	-33.037	1.00	31.37
BBBBATOM	3039	CG	ASP	B	59	-10.766	-52.863	-34.104	1.00	32.68
BBBBATOM	3040	OD1	ASP	B	59	-11.969	-53.037	-33.812	1.00	32.40
BBBBATOM	3041	OD2	ASP	B	59	-10.378	-52.468	-35.224	1.00	33.40
BBBBATOM	3042	C	ASP	B	59	-9.119	-52.950	-30.618	1.00	30.50
BBBBATOM	3043	O	ASP	B	59	-7.987	-52.491	-30.492	1.00	30.24
BBBBATOM	3044	N	PHE	B	60	-9.608	-53.888	-29.815	1.00	30.65
BBBBATOM	3045	CA	PHE	B	60	-8.809	-54.410	-28.713	1.00	30.32
BBBBATOM	3046	CB	PHE	B	60	-9.560	-54.239	-27.385	1.00	30.74
BBBBATOM	3047	CG	PHE	B	60	-9.925	-52.815	-27.058	1.00	32.14
BBBBATOM	3048	CD1	PHE	B	60	-11.250	-52.392	-27.129	1.00	33.15
BBBBATOM	3049	CD2	PHE	B	60	-8.955	-51.908	-26.649	1.00	31.57
BBBBATOM	3050	CE1	PHE	B	60	-11.605	-51.083	-26.791	1.00	34.05
BBBBATOM	3051	CE2	PHE	B	60	-9.294	-50.598	-26.310	1.00	33.00
BBBBATOM	3052	CZ	PHE	B	60	-10.626	-50.185	-26.380	1.00	33.82
BBBBATOM	3053	C	PHE	B	60	-8.430	-55.878	-28.846	1.00	29.86
BBBBATOM	3054	O	PHE	B	60	-9.154	-56.668	-29.445	1.00	29.93
BBBBATOM	3055	N	ILE	B	61	-7.271	-56.229	-28.295	1.00	29.38
BBBBATOM	3056	CA	ILE	B	61	-6.832	-57.616	-28.269	1.00	28.55
BBBBATOM	3057	CB	ILE	B	61	-5.674	-57.923	-29.258	1.00	28.48
BBBBATOM	3058	CG2	ILE	B	61	-6.123	-57.650	-30.694	1.00	27.65
BBBBATOM	3059	CG1	ILE	B	61	-4.422	-57.126	-28.892	1.00	26.70
BBBBATOM	3060	CD1	ILE	B	61	-3.177	-57.615	-29.638	1.00	27.03
BBBBATOM	3061	C	ILE	B	61	-6.344	-57.855	-26.848	1.00	29.13
BBBBATOM	3062	O	ILE	B	61	-6.124	-56.906	-26.091	1.00	28.80

BBBBATOM	3063	N	ARG B	62	-6.186	-59.116	-26.473	1.00	29.38
BBBBATOM	3064	CA	ARG B	62	-5.709	-59.416	-25.133	1.00	30.76
BBBBATOM	3065	CB	ARG B	62	-6.630	-60.447	-24.461	1.00	32.36
BBBBATOM	3066	CG	ARG B	62	-6.130	-60.955	-23.114	1.00	35.99
BBBBATOM	3067	CD	ARG B	62	-5.438	-59.859	-22.311	1.00	37.86
BBBBATOM	3068	NE	ARG B	62	-6.297	-58.718	-22.004	1.00	40.01
BBBBATOM	3069	CZ	ARG B	62	-5.840	-57.504	-21.711	1.00	39.09
BBBBATOM	3070	NH1	ARG B	62	-4.536	-57.275	-21.690	1.00	39.24
BBBBATOM	3071	NH2	ARG B	62	-6.686	-56.518	-21.439	1.00	40.03
BBBBATOM	3072	C	ARG B	62	-4.274	-59.923	-25.156	1.00	29.32
BBBBATOM	3073	O	ARG B	62	-3.933	-60.809	-25.934	1.00	28.65
BBBBATOM	3074	N	ILE B	63	-3.428	-59.342	-24.313	1.00	30.07
BBBBATOM	3075	CA	ILE B	63	-2.036	-59.770	-24.231	1.00	31.38
BBBBATOM	3076	CB	ILE B	63	-1.081	-58.745	-24.883	1.00	30.06
BBBBATOM	3077	CG2	ILE B	63	-1.442	-58.567	-26.353	1.00	30.41
BBBBATOM	3078	CG1	ILE B	63	-1.143	-57.411	-24.137	1.00	29.94
BBBBATOM	3079	CD1	ILE B	63	-0.128	-56.384	-24.632	1.00	29.62
BBBBATOM	3080	C	ILE B	63	-1.623	-59.981	-22.775	1.00	33.08
BBBBATOM	3081	O	ILE B	63	-0.444	-59.872	-22.430	1.00	33.21
BBBBATOM	3082	N	SER B	64	-2.603	-60.284	-21.927	1.00	35.38
BBBBATOM	3083	CA	SER B	64	-2.356	-60.520	-20.505	1.00	37.51
BBBBATOM	3084	CB	SER B	64	-3.652	-60.912	-19.792	1.00	38.82
BBBBATOM	3085	OG	SER B	64	-4.558	-59.823	-19.750	1.00	42.88
BBBBATOM	3086	C	SER B	64	-1.326	-61.622	-20.311	1.00	37.32
BBBBATOM	3087	O	SER B	64	-1.411	-62.682	-20.933	1.00	37.86
BBBBATOM	3088	N	GLY B	65	-0.356	-61.370	-19.441	1.00	37.81
BBBBATOM	3089	CA	GLY B	65	0.679	-62.355	-19.199	1.00	37.13
BBBBATOM	3090	C	GLY B	65	1.798	-62.283	-20.226	1.00	36.76
BBBBATOM	3091	O	GLY B	65	2.858	-62.889	-20.038	1.00	37.57
BBBBATOM	3092	N	LEU B	66	1.577	-61.539	-21.307	1.00	34.63
BBBBATOM	3093	CA	LEU B	66	2.591	-61.413	-22.355	1.00	33.17
BBBBATOM	3094	CB	LEU B	66	1.936	-61.470	-23.735	1.00	32.08
BBBBATOM	3095	CG	LEU B	66	1.162	-62.747	-24.061	1.00	32.52
BBBBATOM	3096	CD1	LEU B	66	0.563	-62.626	-25.445	1.00	31.38
BBBBATOM	3097	CD2	LEU B	66	2.093	-63.957	-23.984	1.00	31.67
BBBBATOM	3098	C	LEU B	66	3.414	-60.133	-22.246	1.00	32.72
BBBBATOM	3099	O	LEU B	66	4.451	-60.002	-22.893	1.00	33.13
BBBBATOM	3100	N	ARG B	67	2.953	-59.185	-21.440	1.00	31.54
BBBBATOM	3101	CA	ARG B	67	3.671	-57.928	-21.277	1.00	30.90
BBBBATOM	3102	CB	ARG B	67	2.888	-56.984	-20.363	1.00	32.28
BBBBATOM	3103	CG	ARG B	67	1.540	-56.576	-20.913	1.00	34.65
BBBBATOM	3104	CD	ARG B	67	0.926	-55.440	-20.097	1.00	36.69
BBBBATOM	3105	NE	ARG B	67	-0.259	-54.889	-20.748	1.00	38.28
BBBBATOM	3106	CZ	ARG B	67	-1.425	-55.519	-20.853	1.00	39.05
BBBBATOM	3107	NH1	ARG B	67	-1.583	-56.734	-20.341	1.00	39.61
BBBBATOM	3108	NH2	ARG B	67	-2.434	-54.935	-21.487	1.00	39.52
BBBBATOM	3109	C	ARG B	67	5.071	-58.142	-20.713	1.00	29.99
BBBBATOM	3110	O	ARG B	67	5.294	-59.034	-19.889	1.00	28.67
BBBBATOM	3111	N	GLY B	68	6.014	-57.321	-21.165	1.00	27.75
BBBBATOM	3112	CA	GLY B	68	7.380	-57.427	-20.685	1.00	26.79
BBBBATOM	3113	C	GLY B	68	8.166	-58.579	-21.280	1.00	25.41
BBBBATOM	3114	O	GLY B	68	9.326	-58.779	-20.943	1.00	26.04
BBBBATOM	3115	N	LYS B	69	7.546	-59.342	-22.170	1.00	24.55
BBBBATOM	3116	CA	LYS B	69	8.238	-60.463	-22.796	1.00	23.93
BBBBATOM	3117	CB	LYS B	69	7.284	-61.641	-23.033	1.00	24.12
BBBBATOM	3118	CG	LYS B	69	6.757	-62.360	-21.794	1.00	25.08
BBBBATOM	3119	CD	LYS B	69	5.887	-63.553	-22.224	1.00	25.44
BBBBATOM	3120	CE	LYS B	69	5.357	-64.358	-21.035	1.00	28.31
BBBBATOM	3121	NZ	LYS B	69	6.468	-64.877	-20.175	1.00	29.71
BBBBATOM	3122	C	LYS B	69	8.825	-60.062	-24.142	1.00	23.32
BBBBATOM	3123	O	LYS B	69	8.151	-59.404	-24.944	1.00	21.96
BBBBATOM	3124	N	GLY B	70	10.075	-60.470	-24.374	1.00	22.48
BBBBATOM	3125	CA	GLY B	70	10.755	-60.229	-25.636	1.00	22.26
BBBBATOM	3126	C	GLY B	70	10.308	-61.337	-26.588	1.00	22.17
BBBBATOM	3127	O	GLY B	70	9.512	-62.183	-26.195	1.00	21.62
BBBBATOM	3128	N	ILE B	71	10.819	-61.373	-27.814	1.00	21.85

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BBBBATOM   3129  CA   ILE  B   71     10.357 -62.386 -28.762  1.00 23.55
BBBBATOM   3130  CB   ILE  B   71     10.926 -62.142 -30.181  1.00 23.52
BBBBATOM   3131  CG2  ILE  B   71     12.435 -62.375 -30.192  1.00 25.96
BBBBATOM   3132  CG1  ILE  B   71     10.264 -63.096 -31.182  1.00 24.18
BBBBATOM   3133  CD1  ILE  B   71      8.745 -62.981 -31.263  1.00 25.73
BBBBATOM   3134  C    ILE  B   71     10.616 -63.840 -28.359  1.00 23.88
BBBBATOM   3135  O    ILE  B   71      9.775 -64.707 -28.592  1.00 21.66
BBBBATOM   3136  N    LYS  B   72     11.764 -64.119 -27.751  1.00 23.82
BBBBATOM   3137  CA   LYS  B   72     12.038 -65.491 -27.343  1.00 24.92
BBBBATOM   3138  CB   LYS  B   72     13.491 -65.634 -26.875  1.00 26.86
BBBBATOM   3139  CG   LYS  B   72     14.496 -65.590 -28.019  1.00 31.29
BBBBATOM   3140  CD   LYS  B   72     15.925 -65.791 -27.518  1.00 36.00
BBBBATOM   3141  CE   LYS  B   72     16.926 -65.816 -28.671  1.00 38.82
BBBBATOM   3142  NZ   LYS  B   72     18.342 -65.957 -28.192  1.00 41.21
BBBBATOM   3143  C    LYS  B   72     11.068 -65.925 -26.245  1.00 23.73
BBBBATOM   3144  O    LYS  B   72     10.592 -67.062 -26.245  1.00 24.08
BBBBATOM   3145  N    ALA  B   73     10.765 -65.016 -25.322  1.00 21.62
BBBBATOM   3146  CA   ALA  B   73      9.839 -65.306 -24.233  1.00 21.18
BBBBATOM   3147  CB   ALA  B   73      9.895 -64.196 -23.187  1.00 22.25
BBBBATOM   3148  C    ALA  B   73      8.412 -65.454 -24.771  1.00 20.36
BBBBATOM   3149  O    ALA  B   73      7.619 -66.250 -24.267  1.00 18.97
BBBBATOM   3150  N    LEU  B   74      8.076 -64.673 -25.791  1.00 20.23
BBBBATOM   3151  CA   LEU  B   74      6.745 -64.762 -26.387  1.00 19.36
BBBBATOM   3152  CB   LEU  B   74      6.540 -63.643 -27.417  1.00 18.42
BBBBATOM   3153  CG   LEU  B   74      6.422 -62.208 -26.884  1.00 18.80
BBBBATOM   3154  CD1  LEU  B   74      6.473 -61.197 -28.039  1.00 19.86
BBBBATOM   3155  CD2  LEU  B   74      5.109 -62.071 -26.104  1.00 19.45
BBBBATOM   3156  C    LEU  B   74      6.549 -66.110 -27.069  1.00 19.37
BBBBATOM   3157  O    LEU  B   74      5.539 -66.779 -26.863  1.00 20.01
BBBBATOM   3158  N    ILE  B   75      7.520 -66.507 -27.883  1.00 20.59
BBBBATOM   3159  CA   ILE  B   75      7.434 -67.768 -28.601  1.00 21.18
BBBBATOM   3160  CB   ILE  B   75      8.571 -67.896 -29.641  1.00 22.95
BBBBATOM   3161  CG2  ILE  B   75      8.334 -69.108 -30.527  1.00 25.38
BBBBATOM   3162  CG1  ILE  B   75      8.598 -66.657 -30.540  1.00 26.82
BBBBATOM   3163  CD1  ILE  B   75      7.304 -66.442 -31.327  1.00 28.48
BBBBATOM   3164  C    ILE  B   75      7.488 -68.942 -27.624  1.00 21.20
BBBBATOM   3165  O    ILE  B   75      7.125 -70.063 -27.979  1.00 21.59
BBBBATOM   3166  N    ALA  B   76      7.940 -68.680 -26.399  1.00 20.49
BBBBATOM   3167  CA   ALA  B   76      7.996 -69.726 -25.374  1.00 21.72
BBBBATOM   3168  CB   ALA  B   76      9.026 -69.372 -24.305  1.00 21.92
BBBBATOM   3169  C    ALA  B   76      6.624 -69.904 -24.732  1.00 21.54
BBBBATOM   3170  O    ALA  B   76      6.441 -70.778 -23.875  1.00 20.75
BBBBATOM   3171  N    ALA  B   77      5.668 -69.066 -25.145  1.00 20.61
BBBBATOM   3172  CA   ALA  B   77      4.289 -69.121 -24.655  1.00 21.07
BBBBATOM   3173  CB   ALA  B   77      3.937 -67.830 -23.924  1.00 20.10
BBBBATOM   3174  C    ALA  B   77      3.383 -69.298 -25.881  1.00 21.69
BBBBATOM   3175  O    ALA  B   77      2.567 -68.430 -26.199  1.00 21.93
BBBBATOM   3176  N    PRO  B   78      3.507 -70.446 -26.564  1.00 22.38
BBBBATOM   3177  CD   PRO  B   78      4.211 -71.603 -25.976  1.00 21.89
BBBBATOM   3178  CA   PRO  B   78      2.772 -70.846 -27.771  1.00 20.95
BBBBATOM   3179  CB   PRO  B   78      3.027 -72.350 -27.861  1.00 22.21
BBBBATOM   3180  CG   PRO  B   78      4.288 -72.547 -27.117  1.00 24.07
BBBBATOM   3181  C    PRO  B   78      1.278 -70.535 -27.813  1.00 21.19
BBBBATOM   3182  O    PRO  B   78      0.789 -69.939 -28.776  1.00 19.68
BBBBATOM   3183  N    LEU  B   79      0.544 -70.961 -26.790  1.00 21.21
BBBBATOM   3184  CA   LEU  B   79     -0.896 -70.728 -26.783  1.00 21.32
BBBBATOM   3185  CB   LEU  B   79     -1.569 -71.476 -25.630  1.00 20.99
BBBBATOM   3186  CG   LEU  B   79     -1.397 -72.988 -25.617  1.00 22.40
BBBBATOM   3187  CD1  LEU  B   79     -2.504 -73.619 -24.772  1.00 22.01
BBBBATOM   3188  CD2  LEU  B   79     -1.438 -73.521 -27.021  1.00 23.82
BBBBATOM   3189  C    LEU  B   79     -1.275 -69.263 -26.707  1.00 21.17
BBBBATOM   3190  O    LEU  B   79     -2.125 -68.800 -27.481  1.00 20.44
BBBBATOM   3191  N    ARG  B   80     -0.656 -68.529 -25.788  1.00 20.91
BBBBATOM   3192  CA   ARG  B   80     -0.980 -67.115 -25.637  1.00 21.30
BBBBATOM   3193  CB   ARG  B   80     -0.444 -66.583 -24.312  1.00 22.12
BBBBATOM   3194  CG   ARG  B   80     -1.286 -67.051 -23.118  1.00 24.03
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BBBBATOM	3195	CD	ARG	B	80	-0.610	-66.738	-21.807	1.00 23.42
BBBBATOM	3196	NE	ARG	B	80	0.581	-67.556	-21.610	1.00 24.59
BBBBATOM	3197	CZ	ARG	B	80	1.466	-67.351	-20.642	1.00 26.08
BBBBATOM	3198	NH1	ARG	B	80	1.290	-66.349	-19.787	1.00 26.92
BBBBATOM	3199	NH2	ARG	B	80	2.514	-68.152	-20.519	1.00 27.22
BBBBATOM	3200	C	ARG	B	80	-0.526	-66.233	-26.790	1.00 21.29
BBBBATOM	3201	O	ARG	B	80	-1.278	-65.355	-27.223	1.00 21.47
BBBBATOM	3202	N	ILE	B	81	0.683	-66.448	-27.303	1.00 19.29
BBBBATOM	3203	CA	ILE	B	81	1.113	-65.621	-28.421	1.00 19.47
BBBBATOM	3204	CB	ILE	B	81	2.639	-65.793	-28.730	1.00 17.92
BBBBATOM	3205	CG2	ILE	B	81	2.949	-67.200	-29.206	1.00 17.33
BBBBATOM	3206	CG1	ILE	B	81	3.067	-64.753	-29.769	1.00 18.63
BBBBATOM	3207	CD1	ILE	B	81	2.746	-63.318	-29.346	1.00 17.46
BBBBATOM	3208	C	ILE	B	81	0.256	-65.937	-29.654	1.00 18.99
BBBBATOM	3209	O	ILE	B	81	-0.149	-65.028	-30.378	1.00 19.38
BBBBATOM	3210	N	PHE	B	82	-0.056	-67.211	-29.880	1.00 19.39
BBBBATOM	3211	CA	PHE	B	82	-0.875	-67.582	-31.038	1.00 19.15
BBBBATOM	3212	CB	PHE	B	82	-1.057	-69.103	-31.136	1.00 19.27
BBBBATOM	3213	CG	PHE	B	82	-1.811	-69.548	-32.368	1.00 19.87
BBBBATOM	3214	CD1	PHE	B	82	-1.180	-69.602	-33.603	1.00 20.87
BBBBATOM	3215	CD2	PHE	B	82	-3.154	-69.898	-32.289	1.00 21.11
BBBBATOM	3216	CE1	PHE	B	82	-1.872	-70.002	-34.753	1.00 21.20
BBBBATOM	3217	CE2	PHE	B	82	-3.857	-70.297	-33.429	1.00 22.26
BBBBATOM	3218	CZ	PHE	B	82	-3.212	-70.349	-34.663	1.00 22.14
BBBBATOM	3219	C	PHE	B	82	-2.250	-66.931	-30.959	1.00 19.94
BBBBATOM	3220	O	PHE	B	82	-2.777	-66.444	-31.970	1.00 19.64
BBBBATOM	3221	N	ASN	B	83	-2.832	-66.923	-29.764	1.00 19.29
BBBBATOM	3222	CA	ASN	B	83	-4.150	-66.332	-29.577	1.00 20.90
BBBBATOM	3223	CB	ASN	B	83	-4.693	-66.641	-28.178	1.00 20.55
BBBBATOM	3224	CG	ASN	B	83	-6.158	-66.244	-28.028	1.00 22.79
BBBBATOM	3225	OD1	ASN	B	83	-6.505	-65.374	-27.229	1.00 25.14
BBBBATOM	3226	ND2	ASN	B	83	-7.018	-66.877	-28.807	1.00 20.47
BBBBATOM	3227	C	ASN	B	83	-4.178	-64.821	-29.812	1.00 20.83
BBBBATOM	3228	O	ASN	B	83	-5.086	-64.316	-30.472	1.00 21.92
BBBBATOM	3229	N	ALA	B	84	-3.203	-64.092	-29.275	1.00 19.74
BBBBATOM	3230	CA	ALA	B	84	-3.177	-62.647	-29.484	1.00 19.30
BBBBATOM	3231	CB	ALA	B	84	-2.060	-62.008	-28.662	1.00 18.59
BBBBATOM	3232	C	ALA	B	84	-2.967	-62.380	-30.981	1.00 19.94
BBBBATOM	3233	O	ALA	B	84	-3.561	-61.459	-31.552	1.00 19.69
BBBBATOM	3234	N	TRP	B	85	-2.118	-63.197	-31.603	1.00 19.77
BBBBATOM	3235	CA	TRP	B	85	-1.820	-63.111	-33.032	1.00 20.56
BBBBATOM	3236	CB	TRP	B	85	-0.754	-64.148	-33.396	1.00 21.46
BBBBATOM	3237	CG	TRP	B	85	-0.365	-64.167	-34.856	1.00 23.00
BBBBATOM	3238	CD2	TRP	B	85	-0.588	-65.232	-35.785	1.00 23.69
BBBBATOM	3239	CE2	TRP	B	85	-0.024	-64.835	-37.022	1.00 24.14
BBBBATOM	3240	CE3	TRP	B	85	-1.206	-66.486	-35.693	1.00 24.79
BBBBATOM	3241	CD1	TRP	B	85	0.301	-63.189	-35.548	1.00 23.17
BBBBATOM	3242	NE1	TRP	B	85	0.509	-63.585	-36.848	1.00 24.28
BBBBATOM	3243	CZ2	TRP	B	85	-0.060	-65.650	-38.160	1.00 24.90
BBBBATOM	3244	CZ3	TRP	B	85	-1.243	-67.299	-36.827	1.00 25.45
BBBBATOM	3245	CH2	TRP	B	85	-0.671	-66.875	-38.045	1.00 25.15
BBBBATOM	3246	C	TRP	B	85	-3.090	-63.354	-33.865	1.00 21.76
BBBBATOM	3247	O	TRP	B	85	-3.339	-62.658	-34.859	1.00 20.40
BBBBATOM	3248	N	ARG	B	86	-3.885	-64.346	-33.467	1.00 22.03
BBBBATOM	3249	CA	ARG	B	86	-5.140	-64.660	-34.166	1.00 23.28
BBBBATOM	3250	CB	ARG	B	86	-5.754	-65.965	-33.623	1.00 24.72
BBBBATOM	3251	CG	ARG	B	86	-4.999	-67.236	-34.021	1.00 27.21
BBBBATOM	3252	CD	ARG	B	86	-5.368	-67.725	-35.418	1.00 29.60
BBBBATOM	3253	NE	ARG	B	86	-6.626	-68.477	-35.422	1.00 31.45
BBBBATOM	3254	CZ	ARG	B	86	-7.185	-69.004	-36.508	1.00 31.37
BBBBATOM	3255	NH1	ARG	B	86	-6.607	-68.862	-37.696	1.00 32.19
BBBBATOM	3256	NH2	ARG	B	86	-8.314	-69.694	-36.405	1.00 31.39
BBBBATOM	3257	C	ARG	B	86	-6.151	-63.517	-34.007	1.00 22.98
BBBBATOM	3258	O	ARG	B	86	-6.890	-63.195	-34.942	1.00 21.37
BBBBATOM	3259	N	GLN	B	87	-6.190	-62.916	-32.821	1.00 22.90
BBBBATOM	3260	CA	GLN	B	87	-7.101	-61.802	-32.567	1.00 24.07

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BBBBATOM	3261	CB	GLN	B	87	-7.046	-61.382	-31.097	1.00 24.33
BBBBATOM	3262	CG	GLN	B	87	-7.873	-62.280	-30.187	1.00 27.24
BBBBATOM	3263	CD	GLN	B	87	-7.720	-61.943	-28.723	1.00 28.81
BBBBATOM	3264	OE1	GLN	B	87	-8.567	-62.296	-27.908	1.00 33.25
BBBBATOM	3265	NE2	GLN	B	87	-6.632	-61.275	-28.375	1.00 29.95
BBBBATOM	3266	C	GLN	B	87	-6.738	-60.618	-33.457	1.00 23.85
BBBBATOM	3267	O	GLN	B	87	-7.613	-60.012	-34.077	1.00 24.02
BBBBATOM	3268	N	ALA	B	88	-5.449	-60.293	-33.521	1.00 23.39
BBBBATOM	3269	CA	ALA	B	88	-4.996	-59.183	-34.355	1.00 23.78
BBBBATOM	3270	CB	ALA	B	88	-3.508	-58.909	-34.116	1.00 23.33
BBBBATOM	3271	C	ALA	B	88	-5.257	-59.485	-35.831	1.00 24.73
BBBBATOM	3272	O	ALA	B	88	-5.655	-58.595	-36.592	1.00 24.72
BBBBATOM	3273	N	ARG	B	89	-5.038	-60.735	-36.244	1.00 24.26
BBBBATOM	3274	CA	ARG	B	89	-5.285	-61.111	-37.636	1.00 24.94
BBBBATOM	3275	CB	ARG	B	89	-4.904	-62.575	-37.893	1.00 25.14
BBBBATOM	3276	CG	ARG	B	89	-3.461	-62.774	-38.353	1.00 24.54
BBBBATOM	3277	CD	ARG	B	89	-3.142	-64.253	-38.510	1.00 25.50
BBBBATOM	3278	NE	ARG	B	89	-3.809	-64.901	-39.641	1.00 24.93
BBBBATOM	3279	CZ	ARG	B	89	-3.329	-64.930	-40.882	1.00 25.90
BBBBATOM	3280	NH1	ARG	B	89	-2.178	-64.336	-41.170	1.00 25.98
BBBBATOM	3281	NH2	ARG	B	89	-3.979	-65.596	-41.831	1.00 26.36
BBBBATOM	3282	C	ARG	B	89	-6.752	-60.909	-38.013	1.00 25.29
BBBBATOM	3283	O	ARG	B	89	-7.056	-60.420	-39.104	1.00 24.27
BBBBATOM	3284	N	ALA	B	90	-7.658	-61.296	-37.118	1.00 24.61
BBBBATOM	3285	CA	ALA	B	90	-9.088	-61.151	-37.383	1.00 26.16
BBBBATOM	3286	CB	ALA	B	90	-9.907	-61.775	-36.254	1.00 25.77
BBBBATOM	3287	C	ALA	B	90	-9.440	-59.673	-37.538	1.00 26.83
BBBBATOM	3288	O	ALA	B	90	-10.213	-59.301	-38.421	1.00 27.71
BBBBATOM	3289	N	ILE	B	91	-8.862	-58.837	-36.685	1.00 26.92
BBBBATOM	3290	CA	ILE	B	91	-9.108	-57.400	-36.733	1.00 26.97
BBBBATOM	3291	CB	ILE	B	91	-8.408	-56.682	-35.565	1.00 27.03
BBBBATOM	3292	CG2	ILE	B	91	-8.327	-55.175	-35.837	1.00 25.82
BBBBATOM	3293	CG1	ILE	B	91	-9.161	-56.962	-34.260	1.00 24.58
BBBBATOM	3294	CD1	ILE	B	91	-8.435	-56.490	-33.021	1.00 24.65
BBBBATOM	3295	C	ILE	B	91	-8.618	-56.787	-38.040	1.00 28.07
BBBBATOM	3296	O	ILE	B	91	-9.289	-55.934	-38.629	1.00 28.41
BBBBATOM	3297	N	MET	B	92	-7.451	-57.227	-38.496	1.00 27.92
BBBBATOM	3298	CA	MET	B	92	-6.872	-56.693	-39.717	1.00 29.03
BBBBATOM	3299	CB	MET	B	92	-5.366	-56.912	-39.712	1.00 27.34
BBBBATOM	3300	CG	MET	B	92	-4.686	-56.235	-38.536	1.00 26.09
BBBBATOM	3301	SD	MET	B	92	-2.919	-56.413	-38.602	1.00 25.72
BBBBATOM	3302	CE	MET	B	92	-2.413	-55.394	-37.218	1.00 24.09
BBBBATOM	3303	C	MET	B	92	-7.488	-57.257	-40.988	1.00 30.07
BBBBATOM	3304	O	MET	B	92	-7.417	-56.628	-42.046	1.00 30.66
BBBBATOM	3305	N	LYS	B	93	-8.082	-58.441	-40.894	1.00 30.96
BBBBATOM	3306	CA	LYS	B	93	-8.735	-59.038	-42.050	1.00 33.20
BBBBATOM	3307	CB	LYS	B	93	-8.969	-60.537	-41.826	1.00 34.31
BBBBATOM	3308	CG	LYS	B	93	-7.689	-61.369	-41.860	1.00 36.71
BBBBATOM	3309	CD	LYS	B	93	-7.956	-62.847	-41.576	1.00 38.43
BBBBATOM	3310	CE	LYS	B	93	-8.781	-63.491	-42.683	1.00 38.82
BBBBATOM	3311	NZ	LYS	B	93	-9.197	-64.881	-42.344	1.00 40.70
BBBBATOM	3312	C	LYS	B	93	-10.067	-58.314	-42.252	1.00 33.65
BBBBATOM	3313	O	LYS	B	93	-10.524	-58.143	-43.382	1.00 34.76
BBBBATOM	3314	N	ALA	B	94	-10.672	-57.877	-41.147	1.00 33.00
BBBBATOM	3315	CA	ALA	B	94	-11.943	-57.157	-41.183	1.00 33.62
BBBBATOM	3316	CB	ALA	B	94	-12.641	-57.260	-39.833	1.00 33.62
BBBBATOM	3317	C	ALA	B	94	-11.752	-55.684	-41.559	1.00 33.95
BBBBATOM	3318	O	ALA	B	94	-12.484	-55.153	-42.397	1.00 33.20
BBBBATOM	3319	N	TYR	B	95	-10.772	-55.028	-40.943	1.00 33.15
BBBBATOM	3320	CA	TYR	B	95	-10.504	-53.620	-41.224	1.00 33.83
BBBBATOM	3321	CB	TYR	B	95	-9.722	-52.992	-40.060	1.00 33.92
BBBBATOM	3322	CG	TYR	B	95	-9.383	-51.525	-40.249	1.00 34.38
BBBBATOM	3323	CD1	TYR	B	95	-10.381	-50.585	-40.499	1.00 36.04
BBBBATOM	3324	CE1	TYR	B	95	-10.071	-49.240	-40.702	1.00 36.49
BBBBATOM	3325	CD2	TYR	B	95	-8.063	-51.082	-40.202	1.00 34.89
BBBBATOM	3326	CE2	TYR	B	95	-7.741	-49.741	-40.401	1.00 35.72

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BBBBATOM   3327  CZ   TYR B  95      -8.750 -48.826 -40.655  1.00 36.79
BBBBATOM   3328  OH   TYR B  95      -8.436 -47.502 -40.874  1.00 37.60
BBBBATOM   3329  C    TYR B  95      -9.743 -53.418 -42.538  1.00 34.06
BBBBATOM   3330  O    TYR B  95      -9.919 -52.404 -43.214  1.00 33.85
BBBBATOM   3331  N    LYS B  96      -8.902 -54.386 -42.896  1.00 33.76
BBBBATOM   3332  CA   LYS B  96      -8.104 -54.327 -44.122  1.00 33.85
BBBBATOM   3333  CB   LYS B  96      -9.004 -54.476 -45.353  1.00 35.14
BBBBATOM   3334  CG   LYS B  96      -9.707 -55.812 -45.463  1.00 37.16
BBBBATOM   3335  CD   LYS B  96     -10.649 -55.843 -46.661  1.00 38.58
BBBBATOM   3336  CE   LYS B  96     -11.388 -57.170 -46.752  1.00 40.07
BBBBATOM   3337  NZ   LYS B  96     -12.319 -57.218 -47.925  1.00 41.29
BBBBATOM   3338  C    LYS B  96      -7.278 -53.049 -44.262  1.00 33.75
BBBBATOM   3339  O    LYS B  96      -7.489 -52.258 -45.189  1.00 34.55
BBBBATOM   3340  N    PRO B  97      -6.326 -52.825 -43.345  1.00 32.59
BBBBATOM   3341  CD   PRO B  97      -6.004 -53.620 -42.143  1.00 32.37
BBBBATOM   3342  CA   PRO B  97      -5.490 -51.623 -43.419  1.00 31.82
BBBBATOM   3343  CB   PRO B  97      -4.850 -51.568 -42.038  1.00 31.66
BBBBATOM   3344  CG   PRO B  97      -4.686 -53.025 -41.704  1.00 31.53
BBBBATOM   3345  C    PRO B  97      -4.458 -51.769 -44.530  1.00 31.60
BBBBATOM   3346  O    PRO B  97      -4.052 -52.881 -44.860  1.00 32.52
BBBBATOM   3347  N    ASP B  98      -4.037 -50.651 -45.112  1.00 31.25
BBBBATOM   3348  CA , ASP B  98      -3.049 -50.685 -46.188  1.00 29.78
BBBBATOM   3349  CB   ASP B  98      -3.234 -49.488 -47.117  1.00 32.00
BBBBATOM   3350  CG   ASP B  98      -4.562 -49.519 -47.837  1.00 34.21
BBBBATOM   3351  OD1  ASP B  98      -5.281 -48.498 -47.795  1.00 35.37
BBBBATOM   3352  OD2  ASP B  98      -4.888 -50.566 -48.443  1.00 35.10
BBBBATOM   3353  C    ASP B  98      -1.654 -50.660 -45.603  1.00 28.70
BBBBATOM   3354  O    ASP B  98      -0.672 -50.973 -46.274  1.00 26.48
BBBBATOM   3355  N    VAL B  99      -1.573 -50.278 -44.337  1.00 26.88
BBBBATOM   3356  CA   VAL B  99      -0.296 -50.214 -43.660  1.00 26.75
BBBBATOM   3357  CB   VAL B  99       0.500 -48.973 -44.132  1.00 27.35
BBBBATOM   3358  CG1  VAL B  99      -0.305 -47.718 -43.867  1.00 29.45
BBBBATOM   3359  CG2  VAL B  99       1.841 -48.908 -43.443  1.00 27.48
BBBBATOM   3360  C    VAL B  99      -0.552 -50.134 -42.162  1.00 25.92
BBBBATOM   3361  O    VAL B  99      -1.585 -49.627 -41.723  1.00 25.04
BBBBATOM   3362  N    VAL B 100       0.374 -50.664 -41.377  1.00 24.63
BBBBATOM   3363  CA   VAL B 100       0.227 -50.613 -39.936  1.00 23.59
BBBBATOM   3364  CB   VAL B 100       0.120 -52.026 -39.327  1.00 24.97
BBBBATOM   3365  CG1  VAL B 100       0.139 -51.941 -37.811  1.00 24.71
BBBBATOM   3366  CG2  VAL B 100      -1.172 -52.683 -39.782  1.00 22.62
BBBBATOM   3367  C    VAL B 100       1.428 -49.881 -39.382  1.00 22.74
BBBBATOM   3368  O    VAL B 100       2.551 -50.093 -39.830  1.00 24.62
BBBBATOM   3369  N    LEU B 101       1.178 -49.001 -38.419  1.00 21.89
BBBBATOM   3370  CA   LEU B 101       2.214 -48.199 -37.797  1.00 21.59
BBBBATOM   3371  CB   LEU B 101       1.823 -46.716 -37.853  1.00 22.86
BBBBATOM   3372  CG   LEU B 101       2.850 -45.580 -37.892  1.00 24.72
BBBBATOM   3373  CD1  LEU B 101       2.237 -44.385 -37.174  1.00 25.30
BBBBATOM   3374  CD2  LEU B 101       4.168 -45.954 -37.273  1.00 24.45
BBBBATOM   3375  C    LEU B 101       2.349 -48.604 -36.336  1.00 20.83
BBBBATOM   3376  O    LEU B 101       1.370 -48.581 -35.595  1.Q0 21.35
BBBBATOM   3377  N    GLY B 102       3.556 -48.986 -35.936  1.00 20.96
BBBBATOM   3378  CA   GLY B 102       3.796 -49.357 -34.549  1.00 19.23
BBBBATOM   3379  C    GLY B 102       4.655 -48.282 -33.918  1.00 18.45
BBBBATOM   3380  O    GLY B 102       5.765 -48.016 -34.381  1.00 18.70
BBBBATOM   3381  N    MET B 103       4.155 -47.660 -32.857  1.00 18.01
BBBBATOM   3382  CA   MET B 103       4.892 -46.597 -32.191  1.00 18.93
BBBBATOM   3383  CB   MET B 103       3.928 -45.477 -31.781  1.00 20.02
BBBBATOM   3384  CG   MET B 103       3.121 -44.888 -32.944  1.00 21.61
BBBBATOM   3385  SD   MET B 103       4.212 -44.135 -34.157  1.00 23.45
BBBBATOM   3386  CE   MET B 103       4.718 -42.680 -33.271  1.00 21.40
BBBBATOM   3387  C    MET B 103       5.612 -47.128 -30.957  1.00 18.98
BBBBATOM   3388  O    MET B 103       6.134 -46.357 -30.158  1.00 17.96
BBBBATOM   3389  N    GLY B 104       5.640 -48.450 -30.827  1.00 21.56
BBBBATOM   3390  CA   GLY B 104       6.275 -49.080 -29.686  1.00 21.89
BBBBATOM   3391  C    GLY B 104       5.192 -49.614 -28.764  1.00 23.28
BBBBATOM   3392  O    GLY B 104       4.009 -49.353 -28.980  1.00 22.50
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BBBBATOM	3393	N	GLY	B	105	5.583	-50.364	-27.741	1.00	23.01
BBBBATOM	3394	CA	GLY	B	105	4.593	-50.905	-26.827	1.00	23.54
BBBBATOM	3395	C	GLY	B	105	4.358	-52.380	-27.078	1.00	23.17
BBBBATOM	3396	O	GLY	B	105	4.449	-52.844	-28.214	1.00	22.69
BBBBATOM	3397	N	TYR	B	106	4.018	-53.118	-26.026	1.00	22.87
BBBBATOM	3398	CA	TYR	B	106	3.818	-54.554	-26.159	1.00	22.37
BBBBATOM	3399	CB	TYR	B	106	3.632	-55.181	-24.774	1.00	25.08
BBBBATOM	3400	CG	TYR	B	106	4.864	-55.008	-23.929	1.00	28.19
BBBBATOM	3401	CD1	TYR	B	106	4.869	-54.153	-22.830	1.00	31.96
BBBBATOM	3402	CE1	TYR	B	106	6.043	-53.915	-22.108	1.00	33.13
BBBBATOM	3403	CD2	TYR	B	106	6.058	-55.631	-24.282	1.00	31.27
BBBBATOM	3404	CE2	TYR	B	106	7.234	-55.400	-23.569	1.00	32.27
BBBBATOM	3405	CZ	TYR	B	106	7.219	-54.541	-22.487	1.00	33.19
BBBBATOM	3406	OH	TYR	B	106	8.388	-54.291	-21.802	1.00	35.95
BBBBATOM	3407	C	TYR	B	106	2.719	-55.018	-27.100	1.00	20.52
BBBBATOM	3408	O	TYR	B	106	2.867	-56.052	-27.746	1.00	20.50
BBBBATOM	3409	N	VAL	B	107	1.628	-54.270	-27.205	1.00	19.06
BBBBATOM	3410	CA	VAL	B	107	0.557	-54.694	-28.099	1.00	18.06
BBBBATOM	3411	CB	VAL	B	107	-0.690	-53.774	-27.978	1.00	20.95
BBBBATOM	3412	CG1	VAL	B	107	-0.407	-52.407	-28.589	1.00	21.39
BBBBATOM	3413	CG2	VAL	B	107	-1.879	-54.433	-28.658	1.00	21.30
BBBBATOM	3414	C	VAL	B	107	1.015	-54.743	-29.559	1.00	17.45
BBBBATOM	3415	O	VAL	B	107	0.502	-55.536	-30.346	1.00	16.99
BBBBATOM	3416	N	SER	B	108	1.991	-53.916	-29.918	1.00	17.96
BBBBATOM	3417	CA	SER	B	108	2.488	-53.892	-31.290	1.00	19.67
BBBBATOM	3418	CB	SER	B	108	3.424	-52.691	-31.508	1.00	19.56
BBBBATOM	3419	OG	SER	B	108	4.666	-52.824	-30.837	1.00	19.63
BBBBATOM	3420	C	SER	B	108	3.197	-55.187	-31.694	1.00	20.38
BBBBATOM	3421	O	SER	B	108	3.385	-55.449	-32.884	1.00	21.25
BBBBATOM	3422	N	GLY	B	109	3.595	-55.995	-30.710	1.00	19.59
BBBBATOM	3423	CA	GLY	B	109	4.251	-57.256	-31.023	1.00	20.03
BBBBATOM	3424	C	GLY	B	109	3.311	-58.170	-31.792	1.00	19.61
BBBBATOM	3425	O	GLY	B	109	3.579	-58.517	-32.940	1.00	19.24
BBBBATOM	3426	N	PRO	B	110	2.206	-58.606	-31.173	1.00	19.20
BBBBATOM	3427	CD	PRO	B	110	1.914	-58.528	-29.729	1.00	19.94
BBBBATOM	3428	CA	PRO	B	110	1.251	-59.478	-31.855	1.00	18.99
BBBBATOM	3429	CB	PRO	B	110	0.198	-59.737	-30.778	1.00	20.41
BBBBATOM	3430	CG	PRO	B	110	0.998	-59.720	-29.515	1.00	19.81
BBBBATOM	3431	C	PRO	B	110	0.651	-58.761	-33.075	1.00	19.22
BBBBATOM	3432	O	PRO	B	110	0.406	-59.371	-34.116	1.00	17.13
BBBBATOM	3433	N	GLY	B	111	0.407	-57.462	-32.927	1.00	19.03
BBBBATOM	3434	CA	GLY	B	111	-0.160	-56.702	-34.025	1.00	19.60
BBBBATOM	3435	C	GLY	B	111	0.764	-56.714	-35.226	1.00	19.59
BBBBATOM	3436	O	GLY	B	111	0.330	-56.979	-36.339	1.00	21.10
BBBBATOM	3437	N	GLY	B	112	2.043	-56.429	-34.995	1.00	19.78
BBBBATOM	3438	CA	GLY	B	112	3.014	-56.417	-36.074	1.00	19.97
BBBBATOM	3439	C	GLY	B	112	3.147	-57.783	-36.724	1.00	20.43
BBBBATOM	3440	O	GLY	B	112	3.233	-57.896	-37.949	1.00	19.94
BBBBATOM	3441	N	LEU	B	113	3.167	-58.828	-35.903	1.00	19.26
BBBBATOM	3442	CA	LEU	B	113	3.265	-60.184	-36.429	1.00	19.49
BBBBATOM	3443	CB	LEU	B	113	3.405	-61.198	-35.289	1.00	18.38
BBBBATOM	3444	CG	LEU	B	113	4.777	-61.270	-34.605	1.00	20.59
BBBBATOM	3445	CD1	LEU	B	113	4.656	-62.059	-33.311	1.00	20.01
BBBBATOM	3446	CD2	LEU	B	113	5.794	-61.914	-35.538	1.00	20.23
BBBBATOM	3447	C	LEU	B	113	2.040	-60.521	-37.274	1.00	18.73
BBBBATOM	3448	O	LEU	B	113	2.143	-61.252	-38.255	1.00	18.44
BBBBATOM	3449	N	ALA	B	114	0.875	-60.010	-36.892	1.00	18.96
BBBBATOM	3450	CA	ALA	B	114	-0.334	-60.292	-37.661	1.00	18.70
BBBBATOM	3451	CB	ALA	B	114	-1.562	-59.855	-36.889	1.00	16.45
BBBBATOM	3452	C	ALA	B	114	-0.288	-59.578	-39.019	1.00	19.30
BBBBATOM	3453	O	ALA	B	114	-0.602	-60.167	-40.052	1.00	20.62
BBBBATOM	3454	N	ALA	B	115	0.082	-58.303	-39.000	1.00	20.57
BBBBATOM	3455	CA	ALA	B	115	0.167	-57.516	-40.229	1.00	21.84
BBBBATOM	3456	CB	ALA	B	115	0.636	-56.108	-39.911	1.00	19.85
BBBBATOM	3457	C	ALA	B	115	1.140	-58.192	-41.189	1.00	21.58
BBBBATOM	3458	O	ALA	B	115	0.815	-58.464	-42.345	1.00	22.14

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BBBBATOM   3459  N    TRP B 116      2.334 -58.476 -40.688  1.00 22.12
BBBBATOM   3460  CA   TRP B 116      3.365 -59.126 -41.478  1.00 23.22
BBBBATOM   3461  CB   TRP B 116      4.584 -59.367 -40.579  1.00 26.08
BBBBATOM   3462  CG   TRP B 116      5.699 -60.136 -41.204  1.00 27.40
BBBBATOM   3463  CD2  TRP B 116      6.168 -61.418 -40.793  1.00 28.77
BBBBATOM   3464  CE2  TRP B 116      7.234 -61.771 -41.655  1.00 30.37
BBBBATOM   3465  CE3  TRP B 116      5.794 -62.308 -39.778  1.00 30.49
BBBBATOM   3466  CD1  TRP B 116      6.473 -59.761 -42.271  1.00 28.30
BBBBATOM   3467  NE1  TRP B 116      7.401 -60.742 -42.547  1.00 29.04
BBBBATOM   3468  CZ2  TRP B 116      7.929 -62.981 -41.529  1.00 31.08
BBBBATOM   3469  CZ3  TRP B 116      6.485 -63.510 -39.653  1.00 31.85
BBBBATOM   3470  CH2  TRP B 116      7.541 -63.834 -40.527  1.00 32.27
BBBBATOM   3471  C    TRP B 116      2.871 -60.434 -42.123  1.00 23.55
BBBBATOM   3472  O    TRP B 116      3.048 -60.643 -43.329  1.00 22.19
BBBBATOM   3473  N    SER B 117      2.231 -61.304 -41.338  1.00 21.35
BBBBATOM   3474  CA   SER B 117      1.735 -62.573 -41.873  1.00 22.61
BBBBATOM   3475  CB   SER B 117      1.167 -63.462 -40.756  1.00 20.72
BBBBATOM   3476  OG   SER B 117      0.010 -62.889 -40.169  1.00 22.72
BBBBATOM   3477  C    SER B 117      0.665 -62.383 -42.940  1.00 23.56
BBBBATOM   3478  O    SER B 117      0.463 -63.262 -43.780  1.00 23.11
BBBBATOM   3479  N    LEU B 118     -0.020 -61.242 -42.905  1.00 24.40
BBBBATOM   3480  CA   LEU B 118     -1.069 -60.957 -43.882  1.00 25.70
BBBBATOM   3481  CB   LEU B 118     -2.195 -60.155 -43.227  1.00 25.80
BBBBATOM   3482  CG   LEU B 118     -3.012 -60.889 -42.159  1.00 26.56
BBBBATOM   3483  CD1  LEU B 118     -3.905 -59.895 -41.433  1.00 26.62
BBBBATOM   3484  CD2  LEU B 118     -3.841 -62.000 -42.801  1.00 26.51
BBBBATOM   3485  C    LEU B 118     -0.539 -60.193 -45.094  1.00 26.87
BBBBATOM   3486  O    LEU B 118     -1.292 -59.878 -46.021  1.00 26.69
BBBBATOM   3487  N    GLY B 119      0.755 -59.898 -45.085  1.00 26.39
BBBBATOM   3488  CA   GLY B 119      1.354 -59.174 -46.192  1.00 27.80
BBBBATOM   3489  C    GLY B 119      1.142 -57.671 -46.120  1.00 27.64
BBBBATOM   3490  O    GLY B 119      1.293 -56.972 -47.122  1.00 28.49
BBBBATOM   3491  N    ILE B 120      0.786 -57.173 -44.940  1.00 25.88
BBBBATOM   3492  CA   ILE B 120      0.568 -55.744 -44.731  1.00 24.85
BBBBATOM   3493  CB   ILE B 120     -0.507 -55.497 -43.652  1.00 24.64
BBBBATOM   3494  CG2  ILE B 120     -0.648 -54.000 -43.397  1.00 24.49
BBBBATOM   3495  CG1  ILE B 120     -1.839 -56.112 -44.093  1.00 24.61
BBBBATOM   3496  CD1  ILE B 120     -2.891 -56.170 -42.991  1.00 23.34
BBBBATOM   3497  C    ILE B 120      1.879 -55.121 -44.272  1.00 24.55
BBBBATOM   3498  O    ILE B 120      2.465 -55.551 -43.275  1.00 23.69
BBBBATOM   3499  N    PRO B 121      2.365 -54.098 -44.995  1.00 23.85
BBBBATOM   3500  CD   PRO B 121      1.780 -53.400 -46.154  1.00 23.64
BBBBATOM   3501  CA   PRO B 121      3.625 -53.477 -44.591  1.00 22.63
BBBBATOM   3502  CB   PRO B 121      3.872 -52.440 -45.691  1.00 23.83
BBBBATOM   3503  CG   PRO B 121      2.485 -52.053 -46.102  1.00 23.96
BBBBATOM   3504  C    PRO B 121      3.583 -52.869 -43.196  1.00 22.21
BBBBATOM   3505  O    PRO B 121      2.617 -52.208 -42.810  1.00 22.46
BBBBATOM   3506  N    VAL B 122      4.641 -53.114 -42.437  1.00 21.69
BBBBATOM   3507  CA   VAL B 122      4.743 -52.594 -41.083  1.00 22.03
BBBBATOM   3508  CB   VAL B 122      5.184 -53.694 -40.095  1.00 21.80
BBBBATOM   3509  CG1  VAL B 122      5.426 -53.085 -38.724  1.00 21.97
BBBBATOM   3510  CG2  VAL B 122      4.133 -54.789 -40.035  1.00 22.19
BBBBATOM   3511  C    VAL B 122      5.754 -51.465 -41.021  1.00 21.29
BBBBATOM   3512  O    VAL B 122      6.892 -51.605 -41.479  1.00 22.83
BBBBATOM   3513  N    VAL B 123      5.330 -50.338 -40.464  1.00 20.94
BBBBATOM   3514  CA   VAL B 123      6.200 -49.184 -40.310  1.00 20.82
BBBBATOM   3515  CB   VAL B 123      5.580 -47.902 -40.932  1.00 22.16
BBBBATOM   3516  CG1  VAL B 123      6.516 -46.722 -40.709  1.00 20.83
BBBBATOM   3517  CG2  VAL B 123      5.322 -48.111 -42.420  1.00 22.66
BBBBATOM   3518  C    VAL B 123      6.338 -48.953 -38.812  1.00 21.09
BBBBATOM   3519  O    VAL B 123      5.341 -48.986 -38.093  1.00 21.48
BBBBATOM   3520  N    LEU B 124      7.557 -48.720 -38.340  1.00 20.53
BBBBATOM   3521  CA   LEU B 124      7.749 -48.485 -36.915  1.00 22.10
BBBBATOM   3522  CB   LEU B 124      8.578 -49.606 -36.286  1.00 22.00
BBBBATOM   3523  CG   LEU B 124      8.160 -51.051 -36.551  1.00 22.45
BBBBATOM   3524  CD1  LEU B 124      9.196 -51.974 -35.905  1.00 23.90
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BBBBATOM	3525	CD2	LEU	B	124	6.765	-51.313	-36.003	1.00	22.34
BBBBATOM	3526	C	LEU	B	124	8.452	-47.172	-36.633	1.00	22.36
BBBBATOM	3527	O	LEU	B	124	9.218	-46.660	-37.461	1.00	20.75
BBBBATOM	3528	N	HIS	B	125	8.182	-46.638	-35.447	1.00	21.40
BBBBATOM	3529	CA	HIS	B	125	8.814	-45.413	-34.981	1.00	21.42
BBBBATOM	3530	CB	HIS	B	125	7.858	-44.218	-35.067	1.00	21.57
BBBBATOM	3531	CG	HIS	B	125	8.432	-42.948	-34.511	1.00	23.73
BBBBATOM	3532	CD2	HIS	B	125	8.300	-42.368	-33.295	1.00	22.15
BBBBATOM	3533	ND1	HIS	B	125	9.274	-42.127	-35.236	1.00	26.23
BBBBATOM	3534	CE1	HIS	B	125	9.631	-41.095	-34.490	1.00	24.20
BBBBATOM	3535	NE2	HIS	B	125	9.054	-41.218	-33.307	1.00	26.07
BBBBATOM	3536	C	HIS	B	125	9.196	-45.642	-33.519	1.00	21.70
BBBBATOM	3537	O	HIS	B	125	8.378	-46.117	-32.725	1.00	19.81
BBBBATOM	3538	N	GLU	B	126	10.444	-45.332	-33.186	1.00	21.20
BBBBATOM	3539	CA	GLU	B	126	10.947	-45.452	-31.817	1.00	22.15
BBBBATOM	3540	CB	GLU	B	126	12.252	-46.246	-31.790	1.00	21.99
BBBBATOM	3541	CG	GLU	B	126	12.958	-46.206	-30.439	1.00	22.04
BBBBATOM	3542	CD	GLU	B	126	12.119	-46.824	-29.338	1.00	21.43
BBBBATOM	3543	OE1	GLU	B	126	11.767	-48.014	-29.471	1.00	21.92
BBBBATOM	3544	OE2	GLU	B	126	11.807	-46.124	-28.349	1.00	21.08
BBBBATOM	3545	C	GLU	B	126	11.205	-44.027	-31.326	1.00	21.93
BBBBATOM	3546	O	GLU	B	126	12.016	-43.300	-31.908	1.00	21.33
BBBBATOM	3547	N	GLN	B	127	10.520	-43.624	-30.259	1.00	22.62
BBBBATOM	3548	CA	GLN	B	127	10.682	-42.270	-29.735	1.00	22.81
BBBBATOM	3549	CB	GLN	B	127	9.414	-41.814	-28.989	1.00	23.56
BBBBATOM	3550	CG	GLN	B	127	8.147	-41.783	-29.830	1.00	24.46
BBBBATOM	3551	CD	GLN	B	127	7.312	-43.041	-29.687	1.00	25.85
BBBBATOM	3552	OE1	GLN	B	127	6.842	-43.366	-28.591	1.00	23.78
BBBBATOM	3553	NE2	GLN	B	127	7.119	-43.758	-30.797	1.00	24.91
BBBBATOM	3554	C	GLN	B	127	11.874	-42.087	-28.809	1.00	22.39
BBBBATOM	3555	O	GLN	B	127	12.399	-40.976	-28.682	1.00	22.43
BBBBATOM	3556	N	ASN	B	128	12.314	-43.173	-28.177	1.00	22.35
BBBBATOM	3557	CA	ASN	B	128	13.406	-43.097	-27.216	1.00	22.96
BBBBATOM	3558	CB	ASN	B	128	13.136	-44.080	-26.064	1.00	22.85
BBBBATOM	3559	CG	ASN	B	128	11.742	-43.919	-25.474	1.00	23.25
BBBBATOM	3560	OD1	ASN	B	128	10.804	-44.632	-25.848	1.00	26.04
BBBBATOM	3561	ND2	ASN	B	128	11.597	-42.975	-24.556	1.00	22.68
BBBBATOM	3562	C	ASN	B	128	14.824	-43.314	-27.742	1.00	23.87
BBBBATOM	3563	O	ASN	B	128	15.026	-43.856	-28.830	1.00	24.05
BBBBATOM	3564	N	GLY	B	129	15.798	-42.885	-26.940	1.00	24.35
BBBBATOM	3565	CA	GLY	B	129	17.203	-43.019	-27.294	1.00	25.36
BBBBATOM	3566	C	GLY	B	129	17.642	-44.468	-27.280	1.00	25.97
BBBBATOM	3567	O	GLY	B	129	18.643	-44.836	-27.891	1.00	25.48
BBBBATOM	3568	N	ILE	B	130	16.886	-45.290	-26.565	1.00	26.18
BBBBATOM	3569	CA	ILE	B	130	17.160	-46.716	-26.488	1.00	28.00
BBBBATOM	3570	CB	ILE	B	130	17.480	-47.145	-25.033	1.00	28.45
BBBBATOM	3571	CG2	ILE	B	130	16.323	-46.785	-24.102	1.00	28.52
BBBBATOM	3572	CG1	ILE	B	130	17.776	-48.642	-24.986	1.00	29.33
BBBBATOM	3573	CD1	ILE	B	130	18.097	-49.149	-23.593	1.00	31.39
BBBBATOM	3574	C	ILE	B	130	15.909	-47.435	-26.999	1.00	27.44
BBBBATOM	3575	O	ILE	B	130	14.793	-47.103	-26.610	1.00	28.58
BBBBATOM	3576	N	ALA	B	131	16.097	-48.405	-27.887	1.00	26.98
BBBBATOM	3577	CA	ALA	B	131	14.978	-49.139	-28.461	1.00	25.88
BBBBATOM	3578	CB	ALA	B	131	15.485	-50.102	-29.525	1.00	25.02
BBBBATOM	3579	C	ALA	B	131	14.171	-49.901	-27.413	1.00	25.20
BBBBATOM	3580	O	ALA	B	131	14.732	-50.544	-26.533	1.00	25.01
BBBBATOM	3581	N	GLY	B	132	12.851	-49.814	-27.506	1.00	24.52
BBBBATOM	3582	CA	GLY	B	132	12.007	-50.532	-26.568	1.00	24.05
BBBBATOM	3583	C	GLY	B	132	12.150	-52.019	-26.831	1.00	23.35
BBBBATOM	3584	O	GLY	B	132	12.582	-52.419	-27.904	1.00	22.89
BBBBATOM	3585	N	LEU	B	133	11.788	-52.846	-25.860	1.00	23.38
BBBBATOM	3586	CA	LEU	B	133	11.903	-54.293	-26.020	1.00	24.54
BBBBATOM	3587	CB	LEU	B	133	11.328	-54.996	-24.786	1.00	25.48
BBBBATOM	3588	CG	LEU	B	133	11.388	-56.527	-24.780	1.00	27.50
BBBBATOM	3589	CD1	LEU	B	133	12.840	-56.984	-24.866	1.00	28.69
BBBBATOM	3590	CD2	LEU	B	133	10.735	-57.059	-23.509	1.00	28.04

BBBBATOM	3591	C	LEU	B	133	11.209	-54.833	-27.276	1.00 22.84
BBBBATOM	3592	O	LEU	B	133	11.784	-55.619	-28.027	1.00 21.86
BBBBATOM	3593	N	THR	B	134	9.975	-54.401	-27.499	1.00 21.72
BBBBATOM	3594	CA	THR	B	134	9.202	-54.860	-28.639	1.00 21.22
BBBBATOM	3595	CB	THR	B	134	7.716	-54.509	-28.449	1.00 20.99
BBBBATOM	3596	OG1	THR	B	134	7.257	-55.075	-27.210	1.00 20.94
BBBBATOM	3597	CG2	THR	B	134	6.872	-55.073	-29.600	1.00 20.64
BBBBATOM	3598	C	THR	B	134	9.693	-54.326	-29.986	1.00 20.62
BBBBATOM	3599	O	THR	B	134	9.843	-55.091	-30.932	1.00 20.33
BBBBATOM	3600	N	ASN	B	135	9.932	-53.021	-30.075	1.00 21.24
BBBBATOM	3601	CA	ASN	B	135	10.407	-52.419	-31.324	1.00 20.50
BBBBATOM	3602	CB	ASN	B	135	10.637	-50.911	-31.142	1.00 19.58
BBBBATOM	3603	CG	ASN	B	135	9.457	-50.058	-31.597	1.00 19.93
BBBBATOM	3604	OD1	ASN	B	135	9.454	-48.837	-31.390	1.00 21.78
BBBBATOM	3605	ND2	ASN	B	135	8.467	-50.677	-32.219	1.00 17.21
BBBBATOM	3606	C	ASN	B	135	11.724	-53.064	-31.767	1.00 20.78
BBBBATOM	3607	O	ASN	B	135	11.945	-53.290	-32.953	1.00 20.41
BBBBATOM	3608	N	LYS	B	136	12.595	-53.366	-30.809	1.00 21.46
BBBBATOM	3609	CA	LYS	B	136	13.886	-53.949	-31.144	1.00 22.79
BBBBATOM	3610	CB	LYS	B	136	14.713	-54.196	-29.879	1.00 24.70
BBBBATOM	3611	CG	LYS	B	136	16.183	-54.424	-30.178	1.00 27.75
BBBBATOM	3612	CD,	LYS	B	136	16.998	-54.494	-28.902	1.00 30.17
BBBBATOM	3613	CE	LYS	B	136	18.479	-54.671	-29.203	1.00 32.33
BBBBATOM	3614	NZ	LYS	B	136	19.278	-54.641	-27.944	1.00 33.37
BBBBATOM	3615	C	LYS	B	136	13.793	-55.229	-31.966	1.00 23.46
BBBBATOM	3616	O	LYS	B	136	14.561	-55.407	-32.912	1.00 23.71
BBBBATOM	3617	N	TRP	B	137	12.868	-56.127	-31.633	1.00 21.78
BBBBATOM	3618	CA	TRP	B	137	12.753	-57.345	-32.424	1.00 22.06
BBBBATOM	3619	CB	TRP	B	137	12.361	-58.552	-31.553	1.00 21.20
BBBBATOM	3620	CG	TRP	B	137	10.990	-58.525	-30.922	1.00 20.23
BBBBATOM	3621	CD2	TRP	B	137	9.748	-58.877	-31.544	1.00 18.68
BBBBATOM	3622	CE2	TRP	B	137	8.743	-58.780	-30.555	1.00 18.97
BBBBATOM	3623	CE3	TRP	B	137	9.383	-59.270	-32.840	1.00 19.75
BBBBATOM	3624	CD1	TRP	B	137	10.696	-58.231	-29.618	1.00 19.62
BBBBATOM	3625	NE1	TRP	B	137	9.349	-58.385	-29.390	1.00 19.31
BBBBATOM	3626	CZ2	TRP	B	137	7.401	-59.058	-30.821	1.00 18.18
BBBBATOM	3627	CZ3	TRP	B	137	8.046	-59.549	-33.107	1.00 18.87
BBBBATOM	3628	CH2	TRP	B	137	7.072	-59.440	-32.099	1.00 18.94
BBBBATOM	3629	C	TRP	B	137	11.768	-57.202	-33.574	1.00 21.75
BBBBATOM	3630	O	TRP	B	137	11.936	-57.822	-34.623	1.00 21.76
BBBBATOM	3631	N	LEU	B	138	10.741	-56.381	-33.386	1.00 21.61
BBBBATOM	3632	CA	LEU	B	138	9.744	-56.188	-34.431	1.00 23.15
BBBBATOM	3633	CB	LEU	B	138	8.618	-55.305	-33.886	1.00 23.87
BBBBATOM	3634	CG	LEU	B	138	7.312	-55.155	-34.664	1.00 26.48
BBBBATOM	3635	CD1	LEU	B	138	6.672	-56.508	-34.915	1.00 25.34
BBBBATOM	3636	CD2	LEU	B	138	6.383	-54.267	-33.851	1.00 25.90
BBBBATOM	3637	C	LEU	B	138	10.384	-55.558	-35.676	1.00 23.07
BBBBATOM	3638	O	LEU	B	138	9.958	-55.801	-36.809	1.00 22.68
BBBBATOM	3639	N	ALA	B	139	11.423	-54.763	-35.453	1.00 23.34
BBBBATOM	3640	CA	ALA	B	139	12.128	-54.092	-36.542	1.00 25.29
BBBBATOM	3641	CB	ALA	B	139	13.298	-53.287	-35.984	1.00 24.97
BBBBATOM	3642	C	ALA	B	139	12.624	-55.064	-37.610	1.00 26.83
BBBBATOM	3643	O	ALA	B	139	12.829	-54.672	-38.754	1.00 27.29
BBBBATOM	3644	N	LYS	B	140	12.801	-56.332	-37.241	1.00 27.38
BBBBATOM	3645	CA	LYS	B	140	13.279	-57.337	-38.182	1.00 28.05
BBBBATOM	3646	CB	LYS	B	140	13.893	-58.501	-37.401	1.00 29.91
BBBBATOM	3647	CG	LYS	B	140	15.134	-58.057	-36.635	1.00 31.62
BBBBATOM	3648	CD	LYS	B	140	15.719	-59.149	-35.757	1.00 33.53
BBBBATOM	3649	CE	LYS	B	140	16.974	-58.634	-35.055	1.00 34.46
BBBBATOM	3650	NZ	LYS	B	140	17.692	-59.713	-34.320	1.00 36.17
BBBBATOM	3651	C	LYS	B	140	12.254	-57.833	-39.212	1.00 27.83
BBBBATOM	3652	O	LYS	B	140	12.602	-58.562	-40.142	1.00 27.80
BBBBATOM	3653	N	ILE	B	141	10.992	-57.445	-39.052	1.00 26.40
BBBBATOM	3654	CA	ILE	B	141	9.963	-57.818	-40.016	1.00 26.09
BBBBATOM	3655	CB	ILE	B	141	8.854	-58.721	-39.405	1.00 26.39
BBBBATOM	3656	CG2	ILE	B	141	9.401	-60.118	-39.145	1.00 28.33

BBBBATOM	3657	CG1	ILE	B	141	8.298	-58.092	-38.127	1.00	26.45
BBBBATOM	3658	CD1	ILE	B	141	7.136	-58.845	-37.549	1.00	26.95
BBBBATOM	3659	C	ILE	B	141	9.316	-56.542	-40.530	1.00	25.81
BBBBATOM	3660	O	ILE	B	141	8.353	-56.586	-41.305	1.00	26.10
BBBBATOM	3661	N	ALA	B	142	9.856	-55.405	-40.097	1.00	23.78
BBBBATOM	3662	CA	ALA	B	142	9.331	-54.107	-40.498	1.00	25.03
BBBBATOM	3663	CB	ALA	B	142	9.717	-53.046	-39.466	1.00	24.89
BBBBATOM	3664	C	ALA	B	142	9.816	-53.680	-41.880	1.00	25.08
BBBBATOM	3665	O	ALA	B	142	10.973	-53.894	-42.237	1.00	24.93
BBBBATOM	3666	N	THR	B	143	8.920	-53.075	-42.651	1.00	25.03
BBBBATOM	3667	CA	THR	B	143	9.262	-52.595	-43.984	1.00	26.10
BBBBATOM	3668	CB	THR	B	143	7.987	-52.318	-44.816	1.00	25.75
BBBBATOM	3669	OG1	THR	B	143	7.249	-53.534	-44.970	1.00	25.54
BBBBATOM	3670	CG2	THR	B	143	8.345	-51.782	-46.207	1.00	26.92
BBBBATOM	3671	C	THR	B	143	10.079	-51.310	-43.863	1.00	26.63
BBBBATOM	3672	O	THR	B	143	10.996	-51.061	-44.656	1.00	27.13
BBBBATOM	3673	N	LYS	B	144	9.753	-50.506	-42.853	1.00	24.95
BBBBATOM	3674	CA	LYS	B	144	10.436	-49.238	-42.618	1.00	24.73
BBBBATOM	3675	CB	LYS	B	144	9.688	-48.103	-43.329	1.00	26.20
BBBBATOM	3676	CG	LYS	B	144	10.202	-46.710	-43.013	1.00	27.44
BBBBATOM	3677	CD	LYS	B	144	11.602	-46.480	-43.558	1.00	29.01
BBBBATOM	3678	CE,	LYS	B	144	12.055	-45.051	-43.293	1.00	29.74
BBBBATOM	3679	NZ	LYS	B	144	13.406	-44.774	-43.854	1.00	31.29
BBBBATOM	3680	C	LYS	B	144	10.506	-48.943	-41.125	1.00	24.61
BBBBATOM	3681	O	LYS	B	144	9.493	-49.008	-40.423	1.00	23.36
BBBBATOM	3682	N	VAL	B	145	11.707	-48.623	-40.656	1.00	23.68
BBBBATOM	3683	CA	VAL	B	145	11.947	-48.311	-39.252	1.00	23.62
BBBBATOM	3684	CB	VAL	B	145	12.981	-49.279	-38.617	1.00	23.66
BBBBATOM	3685	CG1	VAL	B	145	13.083	-49.014	-37.114	1.00	24.44
BBBBATOM	3686	CG2	VAL	B	145	12.589	-50.724	-38.878	1.00	23.51
BBBBATOM	3687	C	VAL	B	145	12.510	-46.900	-39.125	1.00	24.09
BBBBATOM	3688	O	VAL	B	145	13.473	-46.545	-39.808	1.00	23.68
BBBBATOM	3689	N	MET	B	146	11.902	-46.103	-38.251	1.00	23.84
BBBBATOM	3690	CA	MET	B	146	12.338	-44.736	-37.993	1.00	23.15
BBBBATOM	3691	CB	MET	B	146	11.274	-43.729	-38.448	1.00	24.72
BBBBATOM	3692	CG	MET	B	146	11.130	-43.577	-39.970	1.00	21.76
BBBBATOM	3693	SD	MET	B	146	9.649	-42.636	-40.468	1.00	25.05
BBBBATOM	3694	CE	MET	B	146	8.376	-43.846	-40.325	1.00	21.96
BBBBATOM	3695	C	MET	B	146	12.567	-44.593	-36.488	1.00	24.69
BBBBATOM	3696	O	MET	B	146	11.963	-45.311	-35.689	1.00	22.43
BBBBATOM	3697	N	GLN	B	147	13.456	-43.678	-36.112	1.00	23.37
BBBBATOM	3698	CA	GLN	B	147	13.762	-43.418	-34.712	1.00	25.05
BBBBATOM	3699	CB	GLN	B	147	15.067	-44.114	-34.301	1.00	24.99
BBBBATOM	3700	CG	GLN	B	147	16.259	-43.750	-35.169	1.00	26.10
BBBBATOM	3701	CD	GLN	B	147	17.527	-44.508	-34.803	1.00	26.65
BBBBATOM	3702	OE1	GLN	B	147	18.425	-44.671	-35.637	1.00	28.62
BBBBATOM	3703	NE2	GLN	B	147	17.615	-44.966	-33.558	1.00	26.05
BBBBATOM	3704	C	GLN	B	147	13.880	-41.911	-34.515	1.00	26.28
BBBBATOM	3705	O	GLN	B	147	14.292	-41.177	-35.430	1.00	25.02
BBBBATOM	3706	N	ALA	B	148	13.518	-41.452	-33.323	1.00	26.58
BBBBATOM	3707	CA	ALA	B	148	13.559	-40.032	-33.009	1.00	26.88
BBBBATOM	3708	CB	ALA	B	148	12.853	-39.776	-31.685	1.00	26.71
BBBBATOM	3709	C	ALA	B	148	14.983	-39.502	-32.954	1.00	27.88
BBBBATOM	3710	O	ALA	B	148	15.293	-38.463	-33.545	1.00	27.38
BBBBATOM	3711	N	PHE	B	149	15.847	-40.219	-32.242	1.00	27.92
BBBBATOM	3712	CA	PHE	B	149	17.239	-39.820	-32.098	1.00	29.39
BBBBATOM	3713	CB	PHE	B	149	17.596	-39.631	-30.617	1.00	28.95
BBBBATOM	3714	CG	PHE	B	149	16.549	-38.910	-29.821	1.00	28.91
BBBBATOM	3715	CD1	PHE	B	149	15.745	-39.603	-28.929	1.00	27.96
BBBBATOM	3716	CD2	PHE	B	149	16.372	-37.537	-29.957	1.00	29.03
BBBBATOM	3717	CE1	PHE	B	149	14.779	-38.945	-28.178	1.00	28.64
BBBBATOM	3718	CE2	PHE	B	149	15.406	-36.866	-29.211	1.00	30.10
BBBBATOM	3719	CZ	PHE	B	149	14.608	-37.575	-28.317	1.00	29.02
BBBBATOM	3720	C	PHE	B	149	18.153	-40.893	-32.673	1.00	30.03
BBBBATOM	3721	O	PHE	B	149	17.750	-42.036	-32.849	1.00	30.05
BBBBATOM	3722	N	PRO	B	150	19.401	-40.530	-32.991	1.00	31.73

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BBBBATOM	3723	CD	PRO	B	150	20.018	-39.192	-33.018	1.00	32.39
BBBBATOM	3724	CA	PRO	B	150	20.310	-41.541	-33.535	1.00	31.87
BBBBATOM	3725	CB	PRO	B	150	21.418	-40.698	-34.154	1.00	33.07
BBBBATOM	3726	CG	PRO	B	150	21.480	-39.517	-33.238	1.00	33.70
BBBBATOM	3727	C	PRO	B	150	20.809	-42.411	-32.376	1.00	31.93
BBBBATOM	3728	O	PRO	B	150	20.873	-41.945	-31.239	1.00	31.39
BBBBATOM	3729	N	GLY	B	151	21.130	-43.671	-32.651	1.00	31.67
BBBBATOM	3730	CA	GLY	B	151	21.629	-44.537	-31.595	1.00	32.62
BBBBATOM	3731	C	GLY	B	151	20.717	-45.655	-31.112	1.00	32.88
BBBBATOM	3732	O	GLY	B	151	21.206	-46.690	-30.657	1.00	32.98
BBBBATOM	3733	N	ALA	B	152	19.403	-45.458	-31.196	1.00	32.24
BBBBATOM	3734	CA	ALA	B	152	18.447	-46.476	-30.753	1.00	32.71
BBBBATOM	3735	CB	ALA	B	152	17.020	-45.924	-30.817	1.00	31.78
BBBBATOM	3736	C	ALA	B	152	18.582	-47.708	-31.643	1.00	33.00
BBBBATOM	3737	O	ALA	B	152	18.528	-48.842	-31.169	1.00	32.08
BBBBATOM	3738	N	PHE	B	153	18.732	-47.462	-32.941	1.00	33.66
BBBBATOM	3739	CA	PHE	B	153	18.925	-48.506	-33.937	1.00	34.83
BBBBATOM	3740	CB	PHE	B	153	17.734	-48.611	-34.893	1.00	33.64
BBBBATOM	3741	CG	PHE	B	153	16.518	-49.244	-34.289	1.00	32.97
BBBBATOM	3742	CD1	PHE	B	153	15.468	-48.461	-33.823	1.00	31.93
BBBBATOM	3743	CD2	PHE	B	153	16.421	-50.628	-34.184	1.00	32.46
BBBBATOM	3744	CE1	PHE	B	153	14.339	-49.049	-33.265	1.00	32.18
BBBBATOM	3745	CE2	PHE	B	153	15.294	-51.224	-33.626	1.00	31.75
BBBBATOM	3746	CZ	PHE	B	153	14.254	-50.435	-33.166	1.00	31.22
BBBBATOM	3747	C	PHE	B	153	20.155	-48.075	-34.723	1.00	36.90
BBBBATOM	3748	O	PHE	B	153	20.407	-46.878	-34.879	1.00	37.54
BBBBATOM	3749	N	PRO	B	154	20.944	-49.040	-35.220	1.00	38.15
BBBBATOM	3750	CD	PRO	B	154	20.845	-50.482	-34.932	1.00	38.37
BBBBATOM	3751	CA	PRO	B	154	22.158	-48.751	-35.993	1.00	38.97
BBBBATOM	3752	CB	PRO	B	154	22.706	-50.143	-36.302	1.00	39.31
BBBBATOM	3753	CG	PRO	B	154	22.274	-50.941	-35.108	1.00	39.50
BBBBATOM	3754	C	PRO	B	154	21.964	-47.921	-37.266	1.00	39.90
BBBBATOM	3755	O	PRO	B	154	22.697	-46.958	-37.496	1.00	39.89
BBBBATOM	3756	N	ASN	B	155	20.979	-48.280	-38.088	1.00	40.46
BBBBATOM	3757	CA	ASN	B	155	20.765	-47.568	-39.346	1.00	41.08
BBBBATOM	3758	CB	ASN	B	155	21.135	-48.488	-40.510	1.00	43.63
BBBBATOM	3759	CG	ASN	B	155	22.618	-48.753	-40.585	1.00	45.00
BBBBATOM	3760	OD1	ASN	B	155	23.401	-47.861	-40.922	1.00	46.41
BBBBATOM	3761	ND2	ASN	B	155	23.019	-49.978	-40.259	1.00	45.20
BBBBATOM	3762	C	ASN	B	155	19.393	-46.966	-39.627	1.00	40.73
BBBBATOM	3763	O	ASN	B	155	19.145	-46.501	-40.742	1.00	41.01
BBBBATOM	3764	N	ALA	B	156	18.507	-46.956	-38.638	1.00	38.93
BBBBATOM	3765	CA	ALA	B	156	17.170	-46.407	-38.843	1.00	37.55
BBBBATOM	3766	CB	ALA	B	156	16.304	-46.689	-37.618	1.00	37.34
BBBBATOM	3767	C	ALA	B	156	17.209	-44.909	-39.123	1.00	36.36
BBBBATOM	3768	O	ALA	B	156	17.934	-44.171	-38.459	1.00	36.95
BBBBATOM	3769	N	GLU	B	157	16.428	-44.464	-40.107	1.00	35.76
BBBBATOM	3770	CA	GLU	B	157	16.367	-43.044	-40.460	1.00	34.40
BBBBATOM	3771	CB	GLU	B	157	15.375	-42.815	-41.613	1.00	34.84
BBBBATOM	3772	CG	GLU	B	157	15.246	-41.349	-42.055	1.00	34.91
BBBBATOM	3773	CD	GLU	B	157	14.171	-41.123	-43.117	1.00	36.66
BBBBATOM	3774	OE1	GLU	B	157	13.952	-39.951	-43.509	1.00	37.67
BBBBATOM	3775	OE2	GLU	B	157	13.543	-42.107	-43.563	1.00	35.62
BBBBATOM	3776	C	GLU	B	157	15.922	-42.249	-39.231	1.00	33.89
BBBBATOM	3777	O	GLU	B	157	14.941	-42.605	-38.574	1.00	33.04
BBBBATOM	3778	N	VAL	B	158	16.655	-41.185	-38.915	1.00	32.73
BBBBATOM	3779	CA	VAL	B	158	16.337	-40.344	-37.764	1.00	31.16
BBBBATOM	3780	CB	VAL	B	158	17.606	-39.680	-37.202	1.00	31.85
BBBBATOM	3781	CG1	VAL	B	158	17.238	-38.729	-36.073	1.00	31.22
BBBBATOM	3782	CG2	VAL	B	158	18.574	-40.752	-36.708	1.00	31.41
BBBBATOM	3783	C	VAL	B	158	15.352	-39.260	-38.178	1.00	30.27
BBBBATOM	3784	O	VAL	B	158	15.649	-38.445	-39.053	1.00	30.18
BBBBATOM	3785	N	VAL	B	159	14.186	-39.241	-37.544	1.00	28.57
BBBBATOM	3786	CA	VAL	B	159	13.155	-38.265	-37.889	1.00	28.10
BBBBATOM	3787	CB	VAL	B	159	11.942	-38.963	-38.535	1.00	27.81
BBBBATOM	3788	CG1	VAL	B	159	12.365	-39.667	-39.819	1.00	28.61

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BBBBATOM	3789	CG2	VAL	B	159	11.336	-39.962	-37.548	1.00	27.61
BBBBATOM	3790	C	VAL	B	159	12.636	-37.430	-36.725	1.00	27.64
BBBBATOM	3791	O	VAL	B	159	11.757	-36.591	-36.918	1.00	27.97
BBBBATOM	3792	N	GLY	B	160	13.168	-37.662	-35.527	1.00	27.60
BBBBATOM	3793	CA	GLY	B	160	12.724	-36.921	-34.355	1.00	26.93
BBBBATOM	3794	C	GLY	B	160	11.331	-37.312	-33.883	1.00	26.66
BBBBATOM	3795	O	GLY	B	160	10.757	-38.275	-34.384	1.00	26.71
BBBBATOM	3796	N	ASN	B	161	10.797	-36.569	-32.914	1.00	25.68
BBBBATOM	3797	CA	ASN	B	161	9.456	-36.807	-32.375	1.00	25.27
BBBBATOM	3798	CB	ASN	B	161	9.481	-36.963	-30.849	1.00	23.89
BBBBATOM	3799	CG	ASN	B	161	10.042	-38.285	-30.401	1.00	22.91
BBBBATOM	3800	OD1	ASN	B	161	9.600	-39.335	-30.850	1.00	22.70
BBBBATOM	3801	ND2	ASN	B	161	11.017	-38.243	-29.496	1.00	22.71
BBBBATOM	3802	C	ASN	B	161	8.556	-35.618	-32.670	1.00	25.39
BBBBATOM	3803	O	ASN	B	161	9.028	-34.499	-32.821	1.00	25.45
BBBBATOM	3804	N	PRO	B	162	7.241	-35.849	-32.741	1.00	26.08
BBBBATOM	3805	CD	PRO	B	162	6.533	-37.140	-32.710	1.00	25.20
BBBBATOM	3806	CA	PRO	B	162	6.315	-34.747	-33.004	1.00	26.14
BBBBATOM	3807	CB	PRO	B	162	4.952	-35.431	-32.976	1.00	25.76
BBBBATOM	3808	CG	PRO	B	162	5.255	-36.821	-33.430	1.00	26.48
BBBBATOM	3809	C	PRO	B	162	6.455	-33.728	-31.866	1.00	27.00
BBBBATOM	3810	O	PRO	B	162	6.652	-34.102	-30.703	1.00	25.08
BBBBATOM	3811	N	VAL	B	163	6.355	-32.446	-32.203	1.00	27.54
BBBBATOM	3812	CA	VAL	B	163	6.456	-31.379	-31.216	1.00	27.75
BBBBATOM	3813	CB	VAL	B	163	7.748	-30.561	-31.421	1.00	28.81
BBBBATOM	3814	CG1	VAL	B	163	7.839	-29.451	-30.381	1.00	28.20
BBBBATOM	3815	CG2	VAL	B	163	8.958	-31.471	-31.335	1.00	27.87
BBBBATOM	3816	C	VAL	B	163	5.261	-30.440	-31.365	1.00	29.43
BBBBATOM	3817	O	VAL	B	163	4.777	-30.227	-32.476	1.00	28.49
BBBBATOM	3818	N	ARG	B	164	4.790	-29.891	-30.246	1.00	29.93
BBBBATOM	3819	CA	ARG	B	164	3.667	-28.953	-30.246	1.00	32.36
BBBBATOM	3820	CB	ARG	B	164	3.430	-28.411	-28.833	1.00	34.56
BBBBATOM	3821	CG	ARG	B	164	2.967	-29.439	-27.832	1.00	38.34
BBBBATOM	3822	CD	ARG	B	164	3.067	-28.889	-26.417	1.00	41.59
BBBBATOM	3823	NE	ARG	B	164	2.481	-27.555	-26.299	1.00	44.08
BBBBATOM	3824	CZ	ARG	B	164	2.307	-26.919	-25.144	1.00	45.79
BBBBATOM	3825	NH1	ARG	B	164	2.673	-27.499	-24.008	1.00	46.89
BBBBATOM	3826	NH2	ARG	B	164	1.769	-25.705	-25.123	1.00	47.50
BBBBATOM	3827	C	ARG	B	164	3.939	-27.775	-31.187	1.00	31.56
BBBBATOM	3828	O	ARG	B	164	5.031	-27.212	-31.191	1.00	30.03
BBBBATOM	3829	N	THR	B	165	2.928	-27.401	-31.965	1.00	32.06
BBBBATOM	3830	CA	THR	B	165	3.038	-26.307	-32.924	1.00	31.74
BBBBATOM	3831	CB	THR	B	165	1.701	-26.104	-33.678	1.00	32.51
BBBBATOM	3832	OG1	THR	B	165	1.198	-27.375	-34.094	1.00	32.54
BBBBATOM	3833	CG2	THR	B	165	1.907	-25.239	-34.916	1.00	32.14
BBBBATOM	3834	C	THR	B	165	3.445	-24.976	-32.295	1.00	31.49
BBBBATOM	3835	O	THR	B	165	4.236	-24.238	-32.872	1.00	31.48
BBBBATOM	3836	N	ASP	B	166	2.907	-24.664	-31.120	1.00	30.86
BBBBATOM	3837	CA	ASP	B	166	3.252	-23.404	-30.466	1.00	30.64
BBBBATOM	3838	CB	ASP	B	166	2.358	-23.163	-29.242	1.00	33.08
BBBBATOM	3839	CG	ASP	B	166	2.185	-24.400	-28.384	1.00	35.24
BBBBATOM	3840	OD1	ASP	B	166	1.315	-24.373	-27.485	1.00	38.19
BBBBATOM	3841	OD2	ASP	B	166	2.908	-25.393	-28.603	1.00	37.17
BBBBATOM	3842	C	ASP	B	166	4.729	-23.338	-30.084	1.00	28.64
BBBBATOM	3843	O	ASP	B	166	5.321	-22.259	-30.076	1.00	27.92
BBBBATOM	3844	N	VAL	B	167	5.328	-24.485	-29.773	1.00	27.08
BBBBATOM	3845	CA	VAL	B	167	6.746	-24.503	-29.440	1.00	25.91
BBBBATOM	3846	CB	VAL	B	167	7.171	-25.824	-28.757	1.00	25.96
BBBBATOM	3847	CG1	VAL	B	167	8.687	-25.844	-28.586	1.00	24.67
BBBBATOM	3848	CG2	VAL	B	167	6.482	-25.964	-27.396	1.00	26.22
BBBBATOM	3849	C	VAL	B	167	7.548	-24.361	-30.736	1.00	25.54
BBBBATOM	3850	O	VAL	B	167	8.548	-23.642	-30.787	1.00	25.58
BBBBATOM	3851	N	LEU	B	168	7.108	-25.059	-31.778	1.00	26.75
BBBBATOM	3852	CA	LEU	B	168	7.780	-25.002	-33.075	1.00	28.46
BBBBATOM	3853	CB	LEU	B	168	7.085	-25.930	-34.080	1.00	28.40
BBBBATOM	3854	CG	LEU	B	168	7.205	-27.440	-33.890	1.00	28.67

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BBBBATOM	3855	CD1	LEU	B	168	6.254	-28.161	-34.854	1.00 30.19
BBBBATOM	3856	CD2	LEU	B	168	8.647	-27.868	-34.129	1.00 28.82
BBBBATOM	3857	C	LEU	B	168	7.766	-23.584	-33.632	1.00 29.14
BBBBATOM	3858	O	LEU	B	168	8.667	-23.186	-34.369	1.00 29.57
BBBBATOM	3859	N	ALA	B	169	6.741	-22.823	-33.267	1.00 30.35
BBBBATOM	3860	CA	ALA	B	169	6.580	-21.455	-33.756	1.00 31.43
BBBBATOM	3861	CB	ALA	B	169	5.118	-21.030	-33.624	1.00 33.26
BBBBATOM	3862	C	ALA	B	169	7.472	-20.427	-33.078	1.00 32.03
BBBBATOM	3863	O	ALA	B	169	7.562	-19.284	-33.536	1.00 31.95
BBBBATOM	3864	N	LEU	B	170	8.131	-20.824	-31.993	1.00 30.53
BBBBATOM	3865	CA	LEU	B	170	9.002	-19.905	-31.268	1.00 29.60
BBBBATOM	3866	CB	LEU	B	170	9.601	-20.595	-30.041	1.00 28.66
BBBBATOM	3867	CG	LEU	B	170	8.623	-20.954	-28.923	1.00 28.67
BBBBATOM	3868	CD1	LEU	B	170	9.322	-21.845	-27.907	1.00 27.66
BBBBATOM	3869	CD2	LEU	B	170	8.096	-19.675	-28.277	1.00 27.21
BBBBATOM	3870	C	LEU	B	170	10.138	-19.363	-32.127	1.00 29.76
BBBBATOM	3871	O	LEU	B	170	10.670	-20.064	-32.983	1.00 29.07
BBBBATOM	3872	N	PRO	B	171	10.525	-18.099	-31.897	1.00 29.71
BBBBATOM	3873	CD	PRO	B	171	9.874	-17.138	-30.989	1.00 30.67
BBBBATOM	3874	CA	PRO	B	171	11.611	-17.457	-32.642	1.00 30.11
BBBBATOM	3875	CB	PRO	B	171	11.665	-16.054	-32.033	1.00 29.54
BBBBATOM	3876	CG	PRO	B	171	10.261	-15.810	-31.605	1.00 30.96
BBBBATOM	3877	C	PRO	B	171	12.900	-18.226	-32.374	1.00 30.39
BBBBATOM	3878	O	PRO	B	171	12.999	-18.933	-31.363	1.00 30.16
BBBBATOM	3879	N	LEU	B	172	13.883	-18.097	-33.263	1.00 28.62
BBBBATOM	3880	CA	LEU	B	172	15.157	-18.780	-33.062	1.00 28.33
BBBBATOM	3881	CB	LEU	B	172	16.106	-18.557	-34.247	1.00 29.88
BBBBATOM	3882	CG	LEU	B	172	15.800	-19.149	-35.628	1.00 32.18
BBBBATOM	3883	CD1	LEU	B	172	15.593	-20.656	-35.510	1.00 32.75
BBBBATOM	3884	CD2	LEU	B	172	14.573	-18.476	-36.222	1.00 33.92
BBBBATOM	3885	C	LEU	B	172	15.805	-18.206	-31.805	1.00 26.61
BBBBATOM	3886	O	LEU	B	172	15.478	-17.093	-31.388	1.00 26.45
BBBBATOM	3887	N	PRO	B	173	16.735	-18.959	-31.190	1.00 25.73
BBBBATOM	3888	CD	PRO	B	173	17.093	-20.345	-31.550	1.00 24.63
BBBBATOM	3889	CA	PRO	B	173	17.450	-18.550	-29.977	1.00 25.25
BBBBATOM	3890	CB	PRO	B	173	18.512	-19.635	-29.827	1.00 25.04
BBBBATOM	3891	CG	PRO	B	173	17.818	-20.831	-30.309	1.00 24.90
BBBBATOM	3892	C	PRO	B	173	18.066	-17.145	-29.999	1.00 24.24
BBBBATOM	3893	O	PRO	B	173	17.791	-16.337	-29.116	1.00 22.89
BBBBATOM	3894	N	GLN	B	174	18.899	-16.850	-30.995	1.00 24.48
BBBBATOM	3895	CA	GLN	B	174	19.526	-15.527	-31.049	1.00 25.46
BBBBATOM	3896	CB	GLN	B	174	20.384	-15.382	-32.313	1.00 26.10
BBBBATOM	3897	CG	GLN	B	174	21.173	-14.070	-32.382	1.00 26.21
BBBBATOM	3898	CD	GLN	B	174	20.325	-12.883	-32.812	1.00 26.24
BBBBATOM	3899	OE1	GLN	B	174	20.634	-11.732	-32.491	1.00 26.98
BBBBATOM	3900	NE2	GLN	B	174	19.258	-13.154	-33.550	1.00 25.58
BBBBATOM	3901	C	GLN	B	174	18.485	-14.408	-30.981	1.00 25.33
BBBBATOM	3902	O	GLN	B	174	18.646	-13.432	-30.249	1.00 24.63
BBBBATOM	3903	N	GLN	B	175	17.402	-14.555	-31.726	1.00 26.49
BBBBATOM	3904	CA	GLN	B	175	16.365	-13.525	-31.718	1.00 28.47
BBBBATOM	3905	CB	GLN	B	175	15.333	-13.819	-32.809	1.00 29.48
BBBBATOM	3906	CG	GLN	B	175	14.206	-12.805	-32.888	1.00 33.70
BBBBATOM	3907	CD	GLN	B	175	13.324	-13.006	-34.109	1.00 35.20
BBBBATOM	3908	OE1	GLN	B	175	12.247	-12.422	-34.215	1.00 38.98
BBBBATOM	3909	NE2	GLN	B	175	13.785	-13.828	-35.042	1.00 37.92
BBBBATOM	3910	C	GLN	B	175	15.678	-13.430	-30.355	1.00 27.54
BBBBATOM	3911	O	GLN	B	175	15.521	-12.346	-29.796	1.00 26.49
BBBBATOM	3912	N	ARG	B	176	15.288	-14.578	-29.818	1.00 28.19
BBBBATOM	3913	CA	ARG	B	176	14.611	-14.635	-28.525	1.00 29.01
BBBBATOM	3914	CB	ARG	B	176	14.183	-16.088	-28.260	1.00 32.12
BBBBATOM	3915	CG	ARG	B	176	13.783	-16.410	-26.825	1.00 34.95
BBBBATOM	3916	CD	ARG	B	176	12.879	-17.638	-26.779	1.00 36.93
BBBBATOM	3917	NE	ARG	B	176	13.401	-18.749	-27.566	1.00 37.99
BBBBATOM	3918	CZ	ARG	B	176	14.458	-19.480	-27.231	1.00 40.44
BBBBATOM	3919	NH1	ARG	B	176	15.121	-19.233	-26.107	1.00 41.22
BBBBATOM	3920	NH2	ARG	B	176	14.866	-20.451	-28.040	1.00 42.79

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BBBBATOM	3921	C	ARG	B	176	15.449	-14.094	-27.357	1.00	28.58
BBBBATOM	3922	O	ARG	B	176	14.933	-13.414	-26.467	1.00	26.70
BBBBATOM	3923	N	LEU	B	177	16.744	-14.382	-27.384	1.00	28.60
BBBBATOM	3924	CA	LEU	B	177	17.673	-13.970	-26.331	1.00	29.90
BBBBATOM	3925	CB	LEU	B	177	18.729	-15.071	-26.140	1.00	30.05
BBBBATOM	3926	CG	LEU	B	177	18.323	-16.402	-25.484	1.00	31.35
BBBBATOM	3927	CD1	LEU	B	177	16.893	-16.755	-25.807	1.00	31.63
BBBBATOM	3928	CD2	LEU	B	177	19.266	-17.504	-25.948	1.00	30.16
BBBBATOM	3929	C	LEU	B	177	18.384	-12.637	-26.594	1.00	30.48
BBBBATOM	3930	O	LEU	B	177	19.148	-12.161	-25.752	1.00	30.67
BBBBATOM	3931	N	ALA	B	178	18.128	-12.036	-27.752	1.00	31.18
BBBBATOM	3932	CA	ALA	B	178	18.766	-10.776	-28.131	1.00	30.78
BBBBATOM	3933	CB	ALA	B	178	18.238	-10.319	-29.496	1.00	32.30
BBBBATOM	3934	C	ALA	B	178	18.639	-9.636	-27.123	1.00	31.11
BBBBATOM	3935	O	ALA	B	178	17.537	-9.253	-26.726	1.00	30.59
BBBBATOM	3936	N	GLY	B	179	19.792	-9.105	-26.718	1.00	30.45
BBBBATOM	3937	CA	GLY	B	179	19.846	-7.993	-25.784	1.00	30.10
BBBBATOM	3938	C	GLY	B	179	19.392	-8.298	-24.374	1.00	29.54
BBBBATOM	3939	O	GLY	B	179	19.288	-7.405	-23.537	1.00	28.79
BBBBATOM	3940	N	ARG	B	180	19.129	-9.568	-24.101	1.00	29.31
BBBBATOM	3941	CA	ARG	B	180	18.676	-9.965	-22.787	1.00	28.97
BBBBATOM	3942	CB,	ARG	B	180	18.120	-11.391	-22.868	1.00	28.73
BBBBATOM	3943	CG	ARG	B	180	17.281	-11.815	-21.693	1.00	25.80
BBBBATOM	3944	CD	ARG	B	180	16.813	-13.245	-21.869	1.00	24.21
BBBBATOM	3945	NE	ARG	B	180	15.595	-13.363	-22.665	1.00	23.27
BBBBATOM	3946	CZ	ARG	B	180	14.898	-14.489	-22.776	1.00	24.65
BBBBATOM	3947	NH1	ARG	B	180	15.316	-15.579	-22.146	1.00	21.06
BBBBATOM	3948	NH2	ARG	B	180	13.777	-14.529	-23.491	1.00	23.07
BBBBATOM	3949	C	ARG	B	180	19.818	-9.874	-21.769	1.00	30.52
BBBBATOM	3950	O	ARG	B	180	20.916	-10.398	-21.980	1.00	30.32
BBBBATOM	3951	N	GLU	B	181	19.562	-9.171	-20.677	1.00	30.40
BBBBATOM	3952	CA	GLU	B	181	20.545	-9.027	-19.621	1.00	31.79
BBBBATOM	3953	CB	GLU	B	181	21.157	-7.617	-19.650	1.00	34.59
BBBBATOM	3954	CG	GLU	B	181	22.130	-7.422	-20.826	1.00	38.85
BBBBATOM	3955	CD	GLU	B	181	22.659	-6.001	-20.957	1.00	41.19
BBBBATOM	3956	OE1	GLU	B	181	23.274	-5.495	-19.996	1.00	43.24
BBBBATOM	3957	OE2	GLU	B	181	22.467	-5.392	-22.032	1.00	43.11
BBBBATOM	3958	C	GLU	B	181	19.815	-9.307	-18.313	1.00	31.51
BBBBATOM	3959	O	GLU	B	181	18.605	-9.543	-18.313	1.00	33.44
BBBBATOM	3960	N	GLY	B	182	20.535	-9.314	-17.203	1.00	29.65
BBBBATOM	3961	CA	GLY	B	182	19.871	-9.586	-15.943	1.00	27.75
BBBBATOM	3962	C	GLY	B	182	19.989	-11.051	-15.565	1.00	25.32
BBBBATOM	3963	O	GLY	B	182	20.573	-11.830	-16.311	1.00	22.00
BBBBATOM	3964	N	PRO	B	183	19.414	-11.455	-14.423	1.00	23.79
BBBBATOM	3965	CD	PRO	B	183	18.562	-10.609	-13.572	1.00	24.07
BBBBATOM	3966	CA	PRO	B	183	19.450	-12.832	-13.913	1.00	22.93
BBBBATOM	3967	CB	PRO	B	183	18.480	-12.796	-12.727	1.00	23.23
BBBBATOM	3968	CG	PRO	B	183	18.549	-11.381	-12.271	1.00	24.61
BBBBATOM	3969	C	PRO	B	183	19.063	-13.912	-14.905	1.00	21.77
BBBBATOM	3970	O	PRO	B	183	18.117	-13.758	-15.683	1.00	21.04
BBBBATOM	3971	N,	VAL	B	184	19.805	-15.011	-14.867	1.00	19.40
BBBBATOM	3972	CA	VAL	B	184	19.524	-16.146	-15.729	1.00	18.01
BBBBATOM	3973	CB	VAL	B	184	20.597	-17.248	-15.549	1.00	17.45
BBBBATOM	3974	CG1	VAL	B	184	20.171	-18.534	-16.249	1.00	15.59
BBBBATOM	3975	CG2	VAL	B	184	21.931	-16.753	-16.121	1.00	18.46
BBBBATOM	3976	C	VAL	B	184	18.155	-16.650	-15.283	1.00	18.17
BBBBATOM	3977	O	VAL	B	184	17.931	-16.882	-14.092	1.00	16.37
BBBBATOM	3978	N	ARG	B	185	17.244	-16.771	-16.245	1.00	17.91
BBBBATOM	3979	CA	ARG	B	185	15.873	-17.216	-16.011	1.00	17.62
BBBBATOM	3980	CB	ARG	B	185	14.966	-16.622	-17.092	1.00	17.65
BBBBATOM	3981	CG	ARG	B	185	15.036	-15.110	-17.160	1.00	18.62
BBBBATOM	3982	CD	ARG	B	185	14.344	-14.624	-18.420	1.00	20.39
BBBBATOM	3983	NE	ARG	B	185	14.307	-13.173	-18.516	1.00	19.72
BBBBATOM	3984	CZ	ARG	B	185	13.647	-12.520	-19.466	1.00	20.23
BBBBATOM	3985	NH1	ARG	B	185	12.977	-13.197	-20.391	1.00	19.85
BBBBATOM	3986	NH2	ARG	B	185	13.650	-11.197	-19.487	1.00	23.44

BBBBATOM	3987	C	ARG	B	185	15.804	-18.740	-16.037	1.00 16.88
BBBBATOM	3988	O	ARG	B	185	15.971	-19.367	-17.087	1.00 15.75
BBBBATOM	3989	N	VAL	B	186	15.566	-19.326	-14.870	1.00 15.97
BBBBATOM	3990	CA	VAL	B	186	15.508	-20.771	-14.741	1.00 16.47
BBBBATOM	3991	CB	VAL	B	186	16.259	-21.245	-13.476	1.00 15.51
BBBBATOM	3992	CG1	VAL	B	186	16.316	-22.770	-13.448	1.00 17.66
BBBBATOM	3993	CG2	VAL	B	186	17.652	-20.626	-13.430	1.00 16.97
BBBBATOM	3994	C	VAL	B	186	14.076	-21.282	-14.644	1.00 16.41
BBBBATOM	3995	O	VAL	B	186	13.343	-20.920	-13.732	1.00 18.33
BBBBATOM	3996	N	LEU	B	187	13.695	-22.128	-15.588	1.00 15.92
BBBBATOM	3997	CA	LEU	B	187	12.361	-22.710	-15.604	1.00 16.75
BBBBATOM	3998	CB	LEU	B	187	11.813	-22.701	-17.035	1.00 16.85
BBBBATOM	3999	CG	LEU	B	187	10.445	-23.340	-17.276	1.00 18.63
BBBBATOM	4000	CD1	LEU	B	187	9.368	-22.478	-16.625	1.00 19.42
BBBBATOM	4001	CD2	LEU	B	187	10.198	-23.449	-18.783	1.00 19.11
BBBBATOM	4002	C	LEU	B	187	12.450	-24.146	-15.085	1.00 16.85
BBBBATOM	4003	O	LEU	B	187	13.115	-24.982	-15.688	1.00 17.18
BBBBATOM	4004	N	VAL	B	188	11.788	-24.426	-13.964	1.00 18.20
BBBBATOM	4005	CA	VAL	B	188	11.774	-25.775	-13.381	1.00 18.41
BBBBATOM	4006	CB	VAL	B	188	11.902	-25.714	-11.842	1.00 18.98
BBBBATOM	4007	CG1	VAL	B	188	12.088	-27.126	-11.270	1.00 18.50
BBBBATOM	4008	.CG2	VAL	B	188	13.061	-24.818	-11.449	1.00 18.83
BBBBATOM	4009	C	VAL	B	188	10.434	-26.440	-13.739	1.00 19.88
BBBBATOM	4010	O	VAL	B	188	9.371	-25.967	-13.336	1.00 20.39
BBBBATOM	4011	N	VAL	B	189	10.493	-27.532	-14.496	1.00 21.55
BBBBATOM	4012	CA	VAL	B	189	9.298	-28.234	-14.948	1.00 22.11
BBBBATOM	4013	CB	VAL	B	189	9.299	-28.342	-16.488	1.00 22.50
BBBBATOM	4014	CG1	VAL	B	189	8.009	-29.013	-16.981	1.00 22.70
BBBBATOM	4015	CG2	VAL	B	189	9.470	-26.943	-17.101	1.00 21.26
BBBBATOM	4016	C	VAL	B	189	9.191	-29.639	-14.351	1.00 23.90
BBBBATOM	4017	O	VAL	B	189	10.067	-30.478	-14.559	1.00 23.61
BBBBATOM	4018	N	GLY	B	190	8.111	-29.887	-13.615	1.00 25.60
BBBBATOM	4019	CA	GLY	B	190	7.914	-31.188	-12.994	1.00 27.28
BBBBATOM	4020	C	GLY	B	190	6.808	-32.026	-13.604	1.00 29.67
BBBBATOM	4021	O	GLY	B	190	6.668	-33.208	-13.283	1.00 29.86
BBBBATOM	4022	N	GLY	B	191	6.025	-31.430	-14.497	1.00 30.56
BBBBATOM	4023	CA	GLY	B	191	4.935	-32.163	-15.115	1.00 31.94
BBBBATOM	4024	C	GLY	B	191	3.676	-32.104	-14.269	1.00 33.11
BBBBATOM	4025	O	GLY	B	191	3.691	-31.556	-13.165	1.00 32.14
BBBBATOM	4026	N	SER	B	192	2.587	-32.673	-14.779	1.00 34.23
BBBBATOM	4027	CA	SER	B	192	1.313	-32.665	-14.064	1.00 35.91
BBBBATOM	4028	CB	SER	B	192	0.283	-33.532	-14.801	1.00 36.87
BBBBATOM	4029	OG	SER	B	192	0.702	-34.887	-14.877	1.00 39.58
BBBBATOM	4030	C	SER	B	192	1.419	-33.128	-12.609	1.00 36.41
BBBBATOM	4031	O	SER	B	192	0.862	-32.499	-11.714	1.00 35.78
BBBBATOM	4032	N	GLN	B	193	2.134	-34.225	-12.380	1.00 37.60
BBBBATOM	4033	CA	GLN	B	193	2.292	-34.763	-11.033	1.00 38.53
BBBBATOM	4034	CB	GLN	B	193	2.584	-36.263	-11.096	1.00 41.10
BBBBATOM	4035	CG	GLN	B	193	1.501	-37.082	-11.779	1.00 45.38
BBBBATOM	4036	CD	GLN	B	193	0.152	-36.948	-11.099	1.00 47.81
BBBBATOM	4037	OE1	GLN	B	193	-0.484	-35.892	-11.149	1.00 49.50
BBBBATOM	4038	NE2	GLN	B	193	-0.290	-38.023	-10.452	1.00 49.36
BBBBATOM	4039	C	GLN	B	193	3.405	-34.072	-10.260	1.00 37.76
BBBBATOM	4040	O	GLN	B	193	3.458	-34.146	-9.030	1.00 37.02
BBBBATOM	4041	N	GLY	B	194	4.291	-33.398	-10.986	1.00 36.47
BBBBATOM	4042	CA	GLY	B	194	5.398	-32.711	-10.350	1.00 35.02
BBBBATOM	4043	C	GLY	B	194	6.584	-33.630	-10.146	1.00 34.51
BBBBATOM	4044	O	GLY	B	194	6.442	-34.851	-10.191	1.00 34.26
BBBBATOM	4045	N	ALA	B	195	7.761	-33.045	-9.938	1.00 33.54
BBBBATOM	4046	CA	ALA	B	195	8.977	-33.819	-9.709	1.00 33.12
BBBBATOM	4047	CB	ALA	B	195	10.073	-33.387	-10.679	1.00 33.17
BBBBATOM	4048	C	ALA	B	195	9.423	-33.590	-8.267	1.00 32.87
BBBBATOM	4049	O	ALA	B	195	9.955	-32.533	-7.923	1.00 31.47
BBBBATOM	4050	N	ARG	B	196	9.195	-34.592	-7.426	1.00 32.81
BBBBATOM	4051	CA	ARG	B	196	9.538	-34.512	-6.010	1.00 32.63
BBBBATOM	4052	CB	ARG	B	196	9.373	-35.891	-5.361	1.00 35.51

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BBBBATOM	4053	CG	ARG	B	196	10.382	-36.954	-5.830	1.00	39.68
BBBBATOM	4054	CD	ARG	B	196	10.317	-37.224	-7.329	1.00	41.52
BBBBATOM	4055	NE	ARG	B	196	9.007	-37.722	-7.738	1.00	43.02
BBBBATOM	4056	CZ	ARG	B	196	8.661	-37.955	-8.997	1.00	42.91
BBBBATOM	4057	NH1	ARG	B	196	9.527	-37.735	-9.975	1.00	44.39
BBBBATOM	4058	NH2	ARG	B	196	7.449	-38.408	-9.279	1.00	45.18
BBBBATOM	4059	C	ARG	B	196	10.940	-33.977	-5.729	1.00	30.96
BBBBATOM	4060	O	ARG	B	196	11.108	-33.035	-4.957	1.00	29.99
BBBBATOM	4061	N	ILE	B	197	11.942	-34.573	-6.367	1.00	29.47
BBBBATOM	4062	CA	ILE	B	197	13.329	-34.168	-6.164	1.00	28.10
BBBBATOM	4063	CB	ILE	B	197	14.284	-35.109	-6.946	1.00	28.46
BBBBATOM	4064	CG2	ILE	B	197	13.984	-35.041	-8.430	1.00	27.99
BBBBATOM	4065	CG1	ILE	B	197	15.742	-34.749	-6.657	1.00	28.64
BBBBATOM	4066	CD1	ILE	B	197	16.212	-35.158	-5.281	1.00	30.51
BBBBATOM	4067	C	ILE	B	197	13.579	-32.703	-6.554	1.00	27.65
BBBBATOM	4068	O	ILE	B	197	14.378	-32.013	-5.921	1.00	27.21
BBBBATOM	4069	N	LEU	B	198	12.897	-32.223	-7.590	1.00	27.07
BBBBATOM	4070	CA	LEU	B	198	13.069	-30.833	-8.003	1.00	26.58
BBBBATOM	4071	CB	LEU	B	198	12.504	-30.616	-9.412	1.00	25.88
BBBBATOM	4072	CG	LEU	B	198	13.196	-31.408	-10.524	1.00	25.40
BBBBATOM	4073	CD1	LEU	B	198	12.625	-31.007	-11.874	1.00	26.54
BBBBATOM	4074	CD2	LEU	B	198	14.692	-31.146	-10.493	1.00	25.94
BBBBATOM	4075	C	LEU	B	198	12.388	-29.893	-7.006	1.00	26.41
BBBBATOM	4076	O	LEU	B	198	12.930	-28.835	-6.667	1.00	26.35
BBBBATOM	4077	N	ASN	B	199	11.205	-30.274	-6.532	1.00	26.01
BBBBATOM	4078	CA	ASN	B	199	10.497	-29.447	-5.563	1.00	27.07
BBBBATOM	4079	CB	ASN	B	199	9.123	-30.035	-5.238	1.00	26.63
BBBBATOM	4080	CG	ASN	B	199	8.212	-30.050	-6.434	1.00	27.62
BBBBATOM	4081	OD1	ASN	B	199	8.519	-29.434	-7.460	1.00	26.33
BBBBATOM	4082	ND2	ASN	B	199	7.080	-30.749	-6.320	1.00	24.20
BBBBATOM	4083	C	ASN	B	199	11.308	-29.319	-4.282	1.00	27.65
BBBBATOM	4084	O	ASN	B	199	11.207	-28.321	-3.581	1.00	28.19
BBBBATOM	4085	N	GLN	B	200	12.124	-30.328	-3.994	1.00	28.38
BBBBATOM	4086	CA	GLN	B	200	12.955	-30.326	-2.794	1.00	30.10
BBBBATOM	4087	CB	GLN	B	200	13.158	-31.764	-2.301	1.00	31.91
BBBBATOM	4088	CG	GLN	B	200	11.883	-32.453	-1.827	1.00	35.02
BBBBATOM	4089	CD	GLN	B	200	12.056	-33.956	-1.632	1.00	37.49
BBBBATOM	4090	OE1	GLN	B	200	11.204	-34.619	-1.032	1.00	38.76
BBBBATOM	4091	NE2	GLN	B	200	13.155	-34.502	-2.151	1.00	37.28
BBBBATOM	4092	C	GLN	B	200	14.319	-29.675	-3.011	1.00	30.18
BBBBATOM	4093	O	GLN	B	200	14.834	-28.975	-2.135	1.00	31.13
BBBBATOM	4094	N	THR	B	201	14.897	-29.884	-4.187	1.00	28.94
BBBBATOM	4095	CA	THR	B	201	16.215	-29.345	-4.474	1.00	27.34
BBBBATOM	4096	CB	THR	B	201	16.915	-30.181	-5.567	1.00	28.81
BBBBATOM	4097	OG1	THR	B	201	16.988	-31.553	-5.149	1.00	28.92
BBBBATOM	4098	CG2	THR	B	201	18.331	-29.654	-5.817	1.00	28.29
BBBBATOM	4099	C	THR	B	201	16.313	-27.871	-4.869	1.00	25.78
BBBBATOM	4100	O	THR	B	201	17.137	-27.138	-4.331	1.00	24.91
BBBBATOM	4101	N	MET	B	202	15.479	-27.430	-5.800	1.00	24.08
BBBBATOM	4102	CA	MET	B	202	15.567	-26.048	-6.268	1.Q0	23.68
BBBBATOM	4103	CB	MET	B	202	14.558	-25.827	-7.397	1.00	22.29
BBBBATOM	4104	CG	MET	B	202	14.856	-26.685	-8.633	1.00	22.80
BBBBATOM	4105	SD	MET	B	202	16.590	-26.614	-9.190	1.00	25.93
BBBBATOM	4106	CE	MET	B	202	16.814	-24.877	-9.345	1.00	22.63
BBBBATOM	4107	C	MET	B	202	15.489	-24.926	-5.229	1.00	23.47
BBBBATOM	4108	O	MET	B	202	16.189	-23.929	-5.354	1.00	24.40
BBBBATOM	4109	N	PRO	B	203	14.636	-25.059	-4.192	1.00	24.12
BBBBATOM	4110	CD	PRO	B	203	13.518	-25.991	-3.970	1.00	22.27
BBBBATOM	4111	CA	PRO	B	203	14.608	-23.963	-3.220	1.00	23.84
BBBBATOM	4112	CB	PRO	B	203	13.553	-24.424	-2.217	1.00	24.46
BBBBATOM	4113	CG	PRO	B	203	12.593	-25.178	-3.084	1.00	24.04
BBBBATOM	4114	C	PRO	B	203	15.987	-23.731	-2.573	1.00	24.07
BBBBATOM	4115	O	PRO	B	203	16.395	-22.593	-2.343	1.00	23.18
BBBBATOM	4116	N	GLN	B	204	16.706	-24.814	-2.290	1.00	25.26
BBBBATOM	4117	CA	GLN	B	204	18.033	-24.708	-1.684	1.00	26.34
BBBBATOM	4118	CB	GLN	B	204	18.474	-26.078	-1.157	1.00	28.67

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BBBBATOM	4119	CG	GLN	B	204	17.555	-26.626	-0.065	1.00	33.65
BBBBATOM	4120	CD	GLN	B	204	17.885	-28.059	0.328	1.00	37.09
BBBBATOM	4121	OE1	GLN	B	204	18.991	-28.354	0.792	1.00	39.30
BBBBATOM	4122	NE2	GLN	B	204	16.924	-28.960	0.140	1.00	38.32
BBBBATOM	4123	C	GLN	B	204	19.030	-24.177	-2.717	1.00	25.36
BBBBATOM	4124	O	GLN	B	204	19.985	-23.466	-2.385	1.00	24.98
BBBBATOM	4125	N	VAL	B	205	18.806	-24.522	-3.978	1.00	24.46
BBBBATOM	4126	CA	VAL	B	205	19.672	-24.033	-5.043	1.00	24.44
BBBBATOM	4127	CB	VAL	B	205	19.288	-24.634	-6.409	1.00	24.84
BBBBATOM	4128	CG1	VAL	B	205	20.039	-23.906	-7.534	1.00	23.72
BBBBATOM	4129	CG2	VAL	B	205	19.614	-26.110	-6.428	1.00	22.91
BBBBATOM	4130	C	VAL	B	205	19.511	-22.515	-5.110	1.00	23.79
BBBBATOM	4131	O	VAL	B	205	20.487	-21.789	-5.270	1.00	25.25
BBBBATOM	4132	N	ALA	B	206	18.273	-22.044	-4.972	1.00	24.12
BBBBATOM	4133	CA	ALA	B	206	17.980	-20.610	-5.013	1.00	22.84
BBBBATOM	4134	CB	ALA	B	206	16.466	-20.377	-4.908	1.00	21.55
BBBBATOM	4135	C	ALA	B	206	18.700	-19.862	-3.890	1.00	24.09
BBBBATOM	4136	O	ALA	B	206	19.174	-18.740	-4.081	1.00	24.90
BBBBATOM	4137	N	ALA	B	207	18.768	-20.477	-2.713	1.00	25.15
BBBBATOM	4138	CA	ALA	B	207	19.442	-19.857	-1.576	1.00	26.65
BBBBATOM	4139	CB	ALA	B	207	19.260	-20.710	-0.324	1.00	27.83
BBBBATOM	4140	C	ALA	B	207	20.924	-19.686	-1.879	1.00	26.96
BBBBATOM	4141	O	ALA	B	207	21.537	-18.693	-1.493	1.00	27.82
BBBBATOM	4142	N	LYS	B	208	21.498	-20.651	-2.586	1.00	27.19
BBBBATOM	4143	CA	LYS	B	208	22.915	-20.595	-2.919	1.00	28.31
BBBBATOM	4144	CB	LYS	B	208	23.432	-21.989	-3.300	1.00	29.85
BBBBATOM	4145	CG	LYS	B	208	23.030	-23.088	-2.329	1.00	32.97
BBBBATOM	4146	CD	LYS	B	208	23.264	-22.667	-0.886	1.00	35.74
BBBBATOM	4147	CE	LYS	B	208	22.689	-23.689	0.084	1.00	37.28
BBBBATOM	4148	NZ	LYS	B	208	21.227	-23.899	-0.135	1.00	35.29
BBBBATOM	4149	C	LYS	B	208	23.237	-19.624	-4.050	1.00	27.83
BBBBATOM	4150	O	LYS	B	208	24.286	-18.978	-4.033	1.00	27.46
BBBBATOM	4151	N	LEU	B	209	22.341	-19.517	-5.028	1.00	26.04
BBBBATOM	4152	CA	LEU	B	209	22.577	-18.640	-6.171	1.00	25.68
BBBBATOM	4153	CB	LEU	B	209	21.975	-19.268	-7.435	1.00	25.08
BBBBATOM	4154	CG	LEU	B	209	22.534	-20.638	-7.844	1.00	25.01
BBBBATOM	4155	CD1	LEU	B	209	21.797	-21.151	-9.074	1.00	25.67
BBBBATOM	4156	CD2	LEU	B	209	24.029	-20.528	-8.119	1.00	25.13
BBBBATOM	4157	C	LEU	B	209	22.075	-17.200	-6.007	1.00	25.59
BBBBATOM	4158	O	LEU	B	209	22.496	-16.313	-6.742	1.00	25.26
BBBBATOM	4159	N	GLY	B	210	21.185	-16.970	-5.045	1.00	26.27
BBBBATOM	4160	CA	GLY	B	210	20.675	-15.628	-4.804	1.00	26.56
BBBBATOM	4161	C	GLY	B	210	20.238	-14.836	-6.030	1.00	27.75
BBBBATOM	4162	O	GLY	B	210	19.518	-15.349	-6.889	1.00	27.68
BBBBATOM	4163	N	ASP	B	211	20.696	-13.585	-6.105	1.00	27.93
BBBBATOM	4164	CA	ASP	B	211	20.370	-12.647	-7.190	1.00	28.28
BBBBATOM	4165	CB	ASP	B	211	21.011	-11.283	-6.906	1.00	29.89
BBBBATOM	4166	CG	ASP	B	211	20.351	-10.545	-5.768	1.00	31.43
BBBBATOM	4167	OD1	ASP	B	211	20.864	-9.469	-5.398	1.00	32.43
BBBBATOM	4168	OD2	ASP	B	211	19.323	-11.025	-5.249	1.00	33.41
BBBBATOM	4169	C	ASP	B	211	20.768	-13.035	-8.615	1.00	27.77
BBBBATOM	4170	O	ASP	B	211	20.320	-12.397	-9.578	1.00	26.32
BBBBATOM	4171	N	SER	B	212	21.616	-14.048	-8.753	1.00	25.75
BBBBATOM	4172	CA	SER	B	212	22.098	-14.474	-10.067	1.00	25.73
BBBBATOM	4173	CB	SER	B	212	23.331	-15.376	-9.904	1.00	26.63
BBBBATOM	4174	OG	SER	B	212	22.971	-16.596	-9.282	1.00	26.71
BBBBATOM	4175	C	SER	B	212	21.062	-15.185	-10.943	1.00	23.61
BBBBATOM	4176	O	SER	B	212	21.262	-15.334	-12.147	1.00	22.28
BBBBATOM	4177	N	VAL	B	213	19.969	-15.644	-10.344	1.00	23.16
BBBBATOM	4178	CA	VAL	B	213	18.925	-16.308	-11.116	1.00	20.76
BBBBATOM	4179	CB	VAL	B	213	18.952	-17.867	-10.989	1.00	21.69
BBBBATOM	4180	CG1	VAL	B	213	20.318	-18.423	-11.375	1.00	19.84
BBBBATOM	4181	CG2	VAL	B	213	18.564	-18.288	-9.576	1.00	20.36
BBBBATOM	4182	C	VAL	B	213	17.535	-15.871	-10.677	1.00	21.41
BBBBATOM	4183	O	VAL	B	213	17.328	-15.396	-9.554	1.00	20.58
BBBBATOM	4184	N	THR	B	214	16.593	-16.021	-11.595	1.00	19.82

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BBBBATOM	4185	CA	THR	B	214	15.204	-15.726	-11.337	1.00	19.60
BBBBATOM	4186	CB	THR	B	214	14.718	-14.478	-12.126	1.00	21.35
BBBBATOM	4187	OG1	THR	B	214	13.323	-14.273	-11.870	1.00	21.93
BBBBATOM	4188	CG2	THR	B	214	14.983	-14.633	-13.622	1.00	19.52
BBBBATOM	4189	C	THR	B	214	14.543	-17.021	-11.791	1.00	20.24
BBBBATOM	4190	O	THR	B	214	14.803	-17.533	-12.893	1.00	18.70
BBBBATOM	4191	N	ILE	B	215	13.706	-17.569	-10.921	1.00	19.21
BBBBATOM	4192	CA	ILE	B	215	13.076	-18.850	-11.169	1.00	18.75
BBBBATOM	4193	CB	ILE	B	215	13.417	-19.828	-10.008	1.00	18.82
BBBBATOM	4194	CG2	ILE	B	215	12.690	-21.157	-10.194	1.00	19.53
BBBBATOM	4195	CG1	ILE	B	215	14.934	-20.030	-9.931	1.00	19.76
BBBBATOM	4196	CD1	ILE	B	215	15.421	-20.656	-8.600	1.00	19.40
BBBBATOM	4197	C	ILE	B	215	11.568	-18.837	-11.315	1.00	19.26
BBBBATOM	4198	O	ILE	B	215	10.874	-18.025	-10.699	1.00	18.28
BBBBATOM	4199	N	TRP	B	216	11.089	-19.737	-12.167	1.00	18.93
BBBBATOM	4200	CA	TRP	B	216	9.661	-19.973	-12.378	1.00	19.34
BBBBATOM	4201	CB	TRP	B	216	9.222	-19.631	-13.797	1.00	18.97
BBBBATOM	4202	CG	TRP	B	216	7.757	-19.897	-14.065	1.00	20.09
BBBBATOM	4203	CD2	TRP	B	216	7.015	-19.467	-15.211	1.00	19.61
BBBBATOM	4204	CE2	TRP	B	216	5.705	-19.988	-15.085	1.00	19.98
BBBBATOM	4205	CE3	TRP	B	216	7.329	-18.690	-16.333	1.00	19.39
BBBBATOM	4206	CD1	TRP	B	216	6.888	-20.639	-13.303	1.00	19.30
BBBBATOM	4207	NE1	TRP	B	216	5.653	-20.700	-13.914	1.00	20.95
BBBBATOM	4208	CZ2	TRP	B	216	4.713	-19.759	-16.043	1.00	22.06
BBBBATOM	4209	CZ3	TRP	B	216	6.336	-18.459	-17.288	1.00	20.42
BBBBATOM	4210	CH2	TRP	B	216	5.047	-18.993	-17.134	1.00	21.16
BBBBATOM	4211	C	TRP	B	216	9.629	-21.479	-12.176	1.00	19.95
BBBBATOM	4212	O	TRP	B	216	10.114	-22.241	-13.010	1.00	19.91
BBBBATOM	4213	N	HIS	B	217	9.067	-21.897	-11.050	1.00	21.62
BBBBATOM	4214	CA	HIS	B	217	9.015	-23.303	-10.680	1.00	21.06
BBBBATOM	4215	CB	HIS	B	217	9.553	-23.419	-9.242	1.00	20.56
BBBBATOM	4216	CG	HIS	B	217	9.717	-24.824	-8.747	1.00	21.95
BBBBATOM	4217	CD2	HIS	B	217	8.915	-25.910	-8.846	1.00	22.12
BBBBATOM	4218	ND1	HIS	B	217	10.807	-25.219	-8.002	1.00	23.39
BBBBATOM	4219	CE1	HIS	B	217	10.670	-26.490	-7.663	1.00	21.82
BBBBATOM	4220	NE2	HIS	B	217	9.530	-26.933	-8.162	1.00	22.14
BBBBATOM	4221	C	HIS	B	217	7.596	-23.870	-10.795	1.00	21.27
BBBBATOM	4222	O	HIS	B	217	6.655	-23.334	-10.214	1.00	21.69
BBBBATOM	4223	N	GLN	B	218	7.448	-24.940	-11.567	1.00	20.83
BBBBATOM	4224	CA	GLN	B	218	6.149	-25.594	-11.735	1.00	24.30
BBBBATOM	4225	CB	GLN	B	218	5.915	-25.935	-13.206	1.00	23.84
BBBBATOM	4226	CG	GLN	B	218	4.561	-26.558	-13.495	1.00	25.91
BBBBATOM	4227	CD	GLN	B	218	4.637	-28.060	-13.673	1.00	26.52
BBBBATOM	4228	OE1	GLN	B	218	3.757	-28.793	-13.214	1.00	28.05
BBBBATOM	4229	NE2	GLN	B	218	5.680	-28.529	-14.360	1.00	25.20
BBBBATOM	4230	C	GLN	B	218	6.173	-26.854	-10.854	1.00	24.64
BBBBATOM	4231	O	GLN	B	218	6.780	-27.866	-11.199	1.00	25.73
BBBBATOM	4232	N	SER	B	219	5.502	-26.756	-9.709	1.00	26.38
BBBBATOM	4233	CA	SER	B	219	5.463	-27.800	-8.684	1.00	26.73
BBBBATOM	4234	CB	SER	B	219	4.947	-27.188	-7.380	1.00	28.26
BBBBATOM	4235	OG	SER	B	219	3.563	-26.881	-7.488	1.00	26.22
BBBBATOM	4236	C	SER	B	219	4.689	-29.096	-8.914	1.00	27.58
BBBBATOM	4237	O	SER	B	219	5.014	-30.122	-8.320	1.00	26.39
BBBBATOM	4238	N	GLY	B	220	3.662	-29.054	-9.750	1.00	28.58
BBBBATOM	4239	CA	GLY	B	220	2.855	-30.242	-9.961	1.00	30.53
BBBBATOM	4240	C	GLY	B	220	1.596	-30.110	-9.111	1.00	31.96
BBBBATOM	4241	O	GLY	B	220	1.523	-29.248	-8.233	1.00	30.92
BBBBATOM	4242	N	LYS	B	221	0.608	-30.965	-9.358	1.00	33.93
BBBBATOM	4243	CA	LYS	B	221	-0.657	-30.914	-8.628	1.00	35.12
BBBBATOM	4244	CB	LYS	B	221	-1.573	-32.049	-9.094	1.00	37.88
BBBBATOM	4245	CG	LYS	B	221	-2.942	-32.055	-8.427	1.00	40.51
BBBBATOM	4246	CD	LYS	B	221	-3.792	-33.215	-8.934	1.00	42.62
BBBBATOM	4247	CE	LYS	B	221	-5.162	-33.249	-8.260	1.00	43.67
BBBBATOM	4248	NZ	LYS	B	221	-6.002	-34.383	-8.763	1.00	45.38
BBBBATOM	4249	C	LYS	B	221	-0.545	-30.950	-7.103	1.00	35.13
BBBBATOM	4250	O	LYS	B	221	0.110	-31.823	-6.531	1.00	34.60

BBBBATOM	4251	N	GLY	B	222	-1.187	-29.979	-6.461	1.00	34.79
BBBBATOM	4252	CA	GLY	B	222	-1.195	-29.899	-5.011	1.00	35.34
BBBBATOM	4253	C	GLY	B	222	0.111	-29.594	-4.299	1.00	35.61
BBBBATOM	4254	O	GLY	B	222	0.163	-29.678	-3.071	1.00	35.51
BBBBATOM	4255	N	SER	B	223	1.158	-29.234	-5.038	1.00	34.65
BBBBATOM	4256	CA	SER	B	223	2.451	-28.934	-4.418	1.00	33.98
BBBBATOM	4257	CB	SER	B	223	3.552	-29.781	-5.062	1.00	35.02
BBBBATOM	4258	OG	SER	B	223	3.303	-31.168	-4.897	1.00	36.07
BBBBATOM	4259	C	SER	B	223	2.839	-27.454	-4.504	1.00	33.55
BBBBATOM	4260	O	SER	B	223	3.930	-27.063	-4.086	1.00	31.72
BBBBATOM	4261	N	GLN	B	224	1.941	-26.639	-5.044	1.00	33.22
BBBBATOM	4262	CA	GLN	B	224	2.187	-25.208	-5.186	1.00	33.71
BBBBATOM	4263	CB	GLN	B	224	0.954	-24.539	-5.799	1.00	35.45
BBBBATOM	4264	CG	GLN	B	224	1.160	-23.120	-6.337	1.00	37.82
BBBBATOM	4265	CD	GLN	B	224	1.344	-22.076	-5.249	1.00	40.08
BBBBATOM	4266	OE1	GLN	B	224	0.669	-22.111	-4.217	1.00	40.97
BBBBATOM	4267	NE2	GLN	B	224	2.244	-21.124	-5.486	1.00	40.08
BBBBATOM	4268	C	GLN	B	224	2.510	-24.560	-3.840	1.00	33.86
BBBBATOM	4269	O	GLN	B	224	3.512	-23.856	-3.697	1.00	33.38
BBBBATOM	4270	N	GLN	B	225	1.659	-24.814	-2.850	1.00	33.06
BBBBATOM	4271	CA	GLN	B	225	1.823	-24.239	-1.519	1.00	32.32
BBBBATOM	4272	CB	GLN	B	225	0.624	-24.619	-0.640	1.00	35.12
BBBBATOM	4273	CG	GLN	B	225	-0.743	-24.143	-1.151	1.00	36.85
BBBBATOM	4274	CD	GLN	B	225	-1.144	-24.751	-2.495	1.00	39.09
BBBBATOM	4275	OE1	GLN	B	225	-0.914	-25.937	-2.759	1.00	39.42
BBBBATOM	4276	NE2	GLN	B	225	-1.768	-23.937	-3.345	1.00	40.13
BBBBATOM	4277	C	GLN	B	225	3.117	-24.606	-0.788	1.00	30.73
BBBBATOM	4278	O	GLN	B	225	3.766	-23.742	-0.202	1.00	30.36
BBBBATOM	4279	N	SER	B	226	3.494	-25.878	-0.817	1.00	29.26
BBBBATOM	4280	CA	SER	B	226	4.701	-26.309	-0.122	1.00	28.30
BBBBATOM	4281	CB	SER	B	226	4.727	-27.834	0.003	1.00	29.10
BBBBATOM	4282	OG	SER	B	226	4.563	-28.461	-1.254	1.00	32.61
BBBBATOM	4283	C	SER	B	226	5.991	-25.809	-0.771	1.00	26.41
BBBBATOM	4284	O	SER	B	226	6.950	-25.486	-0.073	1.00	25.24
BBBBATOM	4285	N	VAL	B	227	6.019	-25.738	-2.099	1.00	25.21
BBBBATOM	4286	CA	VAL	B	227	7.214	-25.247	-2.791	1.00	24.28
BBBBATOM	4287	CB	VAL	B	227	7.150	-25.527	-4.317	1.00	23.32
BBBBATOM	4288	CG1	VAL	B	227	8.368	-24.914	-5.028	1.00	20.67
BBBBATOM	4289	CG2	VAL	B	227	7.117	-27.024	-4.563	1.00	22.45
BBBBATOM	4290	C	VAL	B	227	7.335	-23.743	-2.545	1.00	24.34
BBBBATOM	4291	O	VAL	B	227	8.421	-23.240	-2.281	1.00	25.50
BBBBATOM	4292	N	GLU	B	228	6.209	-23.035	-2.623	1.00	26.12
BBBBATOM	4293	CA	GLU	B	228	6.178	-21.592	-2.387	1.00	27.23
BBBBATOM	4294	CB	GLU	B	228	4.735	-21.075	-2.476	1.00	28.60
BBBBATOM	4295	CG	GLU	B	228	4.558	-19.586	-2.184	1.00	30.24
BBBBATOM	4296	CD	GLU	B	228	4.938	-18.688	-3.356	1.00	31.99
BBBBATOM	4297	OE1	GLU	B	228	5.012	-17.452	-3.159	1.00	31.68
BBBBATOM	4298	OE2	GLU	B	228	5.154	-19.212	-4.471	1.00	32.04
BBBBATOM	4299	C	GLU	B	228	6.746	-21.327	-0.994	1.00	27.95
BBBBATOM	4300	O	GLU	B	228	7.511	-20.383	-0.787	1.00	27.32
BBBBATOM	4301	N	GLN	B	229	6.374	-22.178	-0.041	1.00	28.66
BBBBATOM	4302	CA	GLN	B	229	6.853	-22.046	1.329	1.00	28.38
BBBBATOM	4303	CB	GLN	B	229	6.082	-22.990	2.261	1.00	31.03
BBBBATOM	4304	CG	GLN	B	229	6.570	-22.946	3.700	1.00	35.48
BBBBATOM	4305	CD	GLN	B	229	5.780	-23.860	4.615	1.00	38.01
BBBBATOM	4306	OE1	GLN	B	229	4.548	-23.810	4.645	1.00	39.26
BBBBATOM	4307	NE2	GLN	B	229	6.484	-24.697	5.370	1.00	38.61
BBBBATOM	4308	C	GLN	B	229	8.338	-22.362	1.407	1.00	27.09
BBBBATOM	4309	O	GLN	B	229	9.084	-21.697	2.124	1.00	28.29
BBBBATOM	4310	N	ALA	B	230	8.771	-23.385	0.677	1.00	26.97
BBBBATOM	4311	CA	ALA	B	230	10.185	-23.754	0.682	1.00	26.18
BBBBATOM	4312	CB	ALA	B	230	10.412	-24.984	-0.184	1.00	25.07
BBBBATOM	4313	C	ALA	B	230	11.054	-22.588	0.192	1.00	26.36
BBBBATOM	4314	O	ALA	B	230	12.119	-22.317	0.755	1.00	25.04
BBBBATOM	4315	N	TYR	B	231	10.605	-21.895	-0.854	1.00	25.85
BBBBATOM	4316	CA	TYR	B	231	11.371	-20.766	-1.366	1.00	25.47

BBBBATOM	4317	CB	TYR	B	231	10.762	-20.248	-2.678	1.00	24.72
BBBBATOM	4318	CG	TYR	B	231	11.236	-21.014	-3.905	1.00	23.66
BBBBATOM	4319	CD1	TYR	B	231	12.546	-20.869	-4.381	1.00	23.97
BBBBATOM	4320	CE1	TYR	B	231	13.006	-21.599	-5.488	1.00	21.40
BBBBATOM	4321	CD2	TYR	B	231	10.393	-21.905	-4.567	1.00	22.63
BBBBATOM	4322	CE2	TYR	B	231	10.841	-22.641	-5.681	1.00	22.71
BBBBATOM	4323	CZ	TYR	B	231	12.151	-22.480	-6.128	1.00	21.91
BBBBATOM	4324	OH	TYR	B	231	12.600	-23.214	-7.199	1.00	21.69
BBBBATOM	4325	C	TYR	B	231	11.450	-19.639	-0.336	1.00	26.53
BBBBATOM	4326	O	TYR	B	231	12.498	-19.011	-0.175	1.00	26.32
BBBBATOM	4327	N	ALA	B	232	10.345	-19.380	0.361	1.00	26.28
BBBBATOM	4328	CA	ALA	B	232	10.342	-18.322	1.368	1.00	27.51
BBBBATOM	4329	CB	ALA	B	232	8.930	-18.109	1.910	1.00	28.09
BBBBATOM	4330	C	ALA	B	232	11.303	-18.695	2.499	1.00	28.03
BBBBATOM	4331	O	ALA	B	232	12.069	-17.858	2.983	1.00	27.93
BBBBATOM	4332	N	GLU	B	233	11.263	-19.958	2.911	1.00	29.43
BBBBATOM	4333	CA	GLU	B	233	12.145	-20.441	3.966	1.00	30.87
BBBBATOM	4334	CB	GLU	B	233	11.772	-21.877	4.344	1.00	33.60
BBBBATOM	4335	CG	GLU	B	233	10.491	-21.973	5.170	1.00	37.67
BBBBATOM	4336	CD	GLU	B	233	10.077	-23.404	5.461	1.00	40.35
BBBBATOM	4337	OE1	GLU	B	233	10.964	-24.283	5.525	1.00	42.97
BBBBATOM	4338	OE2	GLU	B	233	8.864	-23.649	5.641	1.00	41.95
BBBBATOM	4339	C	GLU	B	233	13.606	-20.369	3.530	1.00	30.58
BBBBATOM	4340	O	GLU	B	233	14.499	-20.202	4.359	1.00	30.82
BBBBATOM	4341	N	ALA	B	234	13.850	-20.485	2.227	1.00	29.17
BBBBATOM	4342	CA	ALA	B	234	15.215	-20.417	1.714	1.00	28.48
BBBBATOM	4343	CB	ALA	B	234	15.310	-21.110	0.354	1.00	27.71
BBBBATOM	4344	C	ALA	B	234	15.649	-18.961	1.588	1.00	27.73
BBBBATOM	4345	O	ALA	B	234	16.787	-18.677	1.213	1.00	27.34
BBBBATOM	4346	N	GLY	B	235	14.731	-18.045	1.890	1.00	26.74
BBBBATOM	4347	CA	GLY	B	235	15.033	-16.627	1.815	1.00	26.23
BBBBATOM	4348	C	GLY	B	235	14.946	-16.009	0.426	1.00	26.13
BBBBATOM	4349	O	GLY	B	235	15.483	-14.924	0.198	1.00	25.67
BBBBATOM	4350	N	GLN	B	236	14.284	-16.696	-0.502	1.00	25.36
BBBBATOM	4351	CA	GLN	B	236	14.121	-16.198	-1.870	1.00	25.53
BBBBATOM	4352	CB	GLN	B	236	14.940	-17.043	-2.852	1.00	25.84
BBBBATOM	4353	CG	GLN	B	236	16.436	-17.074	-2.603	1.00	27.18
BBBBATOM	4354	CD	GLN	B	236	17.080	-15.705	-2.661	1.00	28.96
BBBBATOM	4355	OE1	GLN	B	236	16.686	-14.850	-3.456	1.00	30.03
BBBBATOM	4356	NE2	GLN	B	236	18.092	-15.495	-1.829	1.00	29.39
BBBBATOM	4357	C	GLN	B	236	12.641	-16.298	-2.232	1.00	24.12
BBBBATOM	4358	O	GLN	B	236	12.262	-17.002	-3.167	1.00	23.31
BBBBATOM	4359	N	PRO	B	237	11.783	-15.578	-1.497	1.00	24.40
BBBBATOM	4360	CD	PRO	B	237	12.143	-14.580	-0.473	1.00	24.52
BBBBATOM	4361	CA	PRO	B	237	10.336	-15.587	-1.720	1.00	24.65
BBBBATOM	4362	CB	PRO	B	237	9.808	-14.798	-0.527	1.00	25.37
BBBBATOM	4363	CG	PRO	B	237	10.862	-13.773	-0.340	1.00	25.24
BBBBATOM	4364	C	PRO	B	237	9.837	-15.012	-3.043	1.00	25.33
BBBBATOM	4365	O	PRO	B	237	8.720	-15.313	-3.465	1.00	24.93
BBBBATOM	4366	N	GLN	B	238	10.663	-14.197	-3.690	1.00	24.47
BBBBATOM	4367	CA	GLN	B	238	10.277	-13.558	-4.945	1.00	24.29
BBBBATOM	4368	CB	GLN	B	238	11.281	-12.455	-5.306	1.00	23.76
BBBBATOM	4369	CG	GLN	B	238	12.622	-12.945	-5.852	1.00	25.22
BBBBATOM	4370	CD	GLN	B	238	13.535	-13.523	-4.783	1.00	26.90
BBBBATOM	4371	OE1	GLN	B	238	13.188	-13.550	-3.600	1.00	28.05
BBBBATOM	4372	NE2	GLN	B	238	14.712	-13.983	-5.195	1.00	25.61
BBBBATOM	4373	C	GLN	B	238	10.108	-14.489	-6.143	1.00	23.41
BBBBATOM	4374	O	GLN	B	238	9.485	-14.112	-7.139	1.00	20.49
BBBBATOM	4375	N	HIS	B	239	10.655	-15.700	-6.069	1.00	22.66
BBBBATOM	4376	CA	HIS	B	239	10.526	-16.608	-7.201	1.00	22.08
BBBBATOM	4377	CB	HIS	B	239	11.432	-17.829	-7.008	1.00	22.41
BBBBATOM	4378	CG	HIS	B	239	12.891	-17.488	-6.998	1.00	20.93
BBBBATOM	4379	CD2	HIS	B	239	13.869	-17.774	-6.104	1.00	20.09
BBBBATOM	4380	ND1	HIS	B	239	13.488	-16.743	-7.992	1.00	20.30
BBBBATOM	4381	CE1	HIS	B	239	14.769	-16.582	-7.711	1.00	22.38
BBBBATOM	4382	NE2	HIS	B	239	15.025	-17.197	-6.569	1.00	19.62

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BBBBATOM	4383	C	HIS	B	239	9.076	-17.024	-7.433	1.00	22.98
BBBBATOM	4384	O	HIS	B	239	8.293	-17.161	-6.490	1.00	21.86
BBBBATOM	4385	N	LYS	B	240	8.727	-17.209	-8.703	1.00	21.76
BBBBATOM	4386	CA	LYS	B	240	7.375	-17.589	-9.105	1.00	23.26
BBBBATOM	4387	CB	LYS	B	240	7.112	-17.102	-10.534	1.00	23.38
BBBBATOM	4388	CG	LYS	B	240	5.718	-17.385	-11.079	1.00	24.06
BBBBATOM	4389	CD	LYS	B	240	5.701	-17.155	-12.585	1.00	23.93
BBBBATOM	4390	CE	LYS	B	240	4.315	-17.309	-13.193	1.00	23.72
BBBBATOM	4391	NZ	LYS	B	240	3.478	-16.129	-12.884	1.00	21.82
BBBBATOM	4392	C	LYS	B	240	7.149	-19.091	-9.046	1.00	23.38
BBBBATOM	4393	O	LYS	B	240	7.922	-19.871	-9.607	1.00	23.06
BBBBATOM	4394	N	VAL	B	241	6.075	-19.497	-8.378	1.00	23.98
BBBBATOM	4395	CA	VAL	B	241	5.740	-20.911	-8.277	1.00	23.78
BBBBATOM	4396	CB	VAL	B	241	5.858	-21.428	-6.833	1.00	24.03
BBBBATOM	4397	CG1	VAL	B	241	5.548	-22.923	-6.803	1.00	24.14
BBBBATOM	4398	CG2	VAL	B	241	7.242	-21.144	-6.281	1.00	23.49
BBBBATOM	4399	C	VAL	B	241	4.299	-21.136	-8.723	1.00	24.15
BBBBATOM	4400	O	VAL	B	241	3.380	-20.528	-8.184	1.00	24.63
BBBBATOM	4401	N	THR	B	242	4.103	-22.000	-9.710	1.00	24.22
BBBBATOM	4402	CA	THR	B	242	2.758	-22.301	-10.177	1.00	25.93
BBBBATOM	4403	CB	THR	B	242	2.513	-21.812	-11.615	1.00	25.89
BBBBATOM	4404	OG1	THR	B	242	3.466	-22.419	-12.492	1.00	27.48
BBBBATOM	4405	CG2	THR	B	242	2.639	-20.299	-11.697	1.00	26.82
BBBBATOM	4406	C	THR	B	242	2.555	-23.809	-10.135	1.00	26.29
BBBBATOM	4407	O	THR	B	242	3.503	-24.577	-10.303	1.00	26.75
BBBBATOM	4408	N	GLU	B	243	1.319	-24.228	-9.898	1.00	26.70
BBBBATOM	4409	CA	GLU	B	243	0.999	-25.651	-9.837	1.00	27.03
BBBBATOM	4410	CB	GLU	B	243	-0.473	-25.828	-9.445	1.00	29.00
BBBBATOM	4411	CG	GLU	B	243	-0.831	-27.218	-8.962	1.00	30.88
BBBBATOM	4412	CD	GLU	B	243	-2.297	-27.341	-8.583	1.00	33.00
BBBBATOM	4413	OE1	GLU	B	243	-2.682	-28.402	-8.048	1.00	33.66
BBBBATOM	4414	OE2	GLU	B	243	-3.063	-26.383	-8.827	1.00	32.17
BBBBATOM	4415	C	GLU	B	243	1.256	-26.289	-11.202	1.00	26.61
BBBBATOM	4416	O	GLU	B	243	1.841	-27.370	-11.304	1.00	26.48
BBBBATOM	4417	N	PHE	B	244	0.807	-25.602	-12.248	1.00	26.54
BBBBATOM	4418	CA	PHE	B	244	0.964	-26.068	-13.620	1.00	26.54
BBBBATOM	4419	CB	PHE	B	244	-0.376	-26.553	-14.186	1.00	29.14
BBBBATOM	4420	CG	PHE	B	244	-1.110	-27.531	-13.307	1.00	30.15
BBBBATOM	4421	CD1	PHE	B	244	-0.622	-28.817	-13.107	1.00	32.26
BBBBATOM	4422	CD2	PHE	B	244	-2.318	-27.172	-12.716	1.00	31.10
BBBBATOM	4423	CE1	PHE	B	244	-1.335	-29.744	-12.328	1.00	33.63
BBBBATOM	4424	CE2	PHE	B	244	-3.040	-28.083	-11.938	1.00	32.04
BBBBATOM	4425	CZ	PHE	B	244	-2.549	-29.371	-11.744	1.00	32.59
BBBBATOM	4426	C	PHE	B	244	1.420	-24.915	-14.507	1.00	25.60
BBBBATOM	4427	O	PHE	B	244	1.604	-23.794	-14.053	1.00	24.93
BBBBATOM	4428	N	ILE	B	245	1.591	-25.223	-15.786	1.00	27.02
BBBBATOM	4429	CA	ILE	B	245	1.932	-24.242	-16.802	1.00	28.48
BBBBATOM	4430	CB	ILE	B	245	3.441	-24.226	-17.159	1.00	28.41
BBBBATOM	4431	CG2	ILE	B	245	3.676	-23.348	-18.399	1.00	27.05
BBBBATOM	4432	CG1	ILE	B	245	4.245	-23.663	-15.983	1.Q0	27.10
BBBBATOM	4433	CD1	ILE	B	245	5.734	-23.543	-16.256	1.00	27.28
BBBBATOM	4434	C	ILE	B	245	1.127	-24.721	-18.000	1.00	30.75
BBBBATOM	4435	O	ILE	B	245	1.428	-25.753	-18.595	1.00	31.41
BBBBATOM	4436	N	ASP	B	246	0.071	-23.997	-18.331	1.00	33.46
BBBBATOM	4437	CA	ASP	B	246	-0.754	-24.396	-19.457	1.00	36.00
BBBBATOM	4438	CB	ASP	B	246	-2.143	-23.754	-19.342	1.00	39.42
BBBBATOM	4439	CG	ASP	B	246	-2.083	-22.246	-19.141	1.00	42.83
BBBBATOM	4440	OD1	ASP	B	246	-1.447	-21.795	-18.162	1.00	44.54
BBBBATOM	4441	OD2	ASP	B	246	-2.678	-21.511	-19.962	1.00	45.41
BBBBATOM	4442	C	ASP	B	246	-0.088	-24.020	-20.780	1.00	35.70
BBBBATOM	4443	O	ASP	B	246	-0.155	-24.768	-21.758	1.00	38.58
BBBBATOM	4444	N	ASP	B	247	0.582	-22.876	-20.794	1.00	33.18
BBBBATOM	4445	CA	ASP	B	247	1.245	-22.392	-21.999	1.00	30.74
BBBBATOM	4446	CB	ASP	B	247	0.936	-20.904	-22.182	1.00	29.62
BBBBATOM	4447	CG	ASP	B	247	1.344	-20.380	-23.548	1.00	30.15
BBBBATOM	4448	OD1	ASP	B	247	2.161	-21.036	-24.225	1.00	27.57

BBBBATOM	4449	OD2	ASP	B	247	0.854	-19.296	-23.935	1.00 29.19
BBBBATOM	4450	C	ASP	B	247	2.754	-22.607	-21.892	1.00 28.87
BBBBATOM	4451	O	ASP	B	247	3.494	-21.695	-21.525	1.00 27.28
BBBBATOM	4452	N	MET	B	248	3.204	-23.818	-22.205	1.00 27.72
BBBBATOM	4453	CA	MET	B	248	4.625	-24.136	-22.138	1.00 28.41
BBBBATOM	4454	CB	MET	B	248	4.856	-25.623	-22.405	1.00 29.48
BBBBATOM	4455	CG	MET	B	248	4.952	-26.469	-21.150	1.00 34.21
BBBBATOM	4456	SD	MET	B	248	6.277	-25.936	-20.049	1.00 38.21
BBBBATOM	4457	CE	MET	B	248	5.611	-26.499	-18.479	1.00 37.90
BBBBATOM	4458	C	MET	B	248	5.429	-23.313	-23.132	1.00 27.22
BBBBATOM	4459	O	MET	B	248	6.578	-22.965	-22.873	1.00 27.06
BBBBATOM	4460	N	ALA	B	249	4.827	-23.009	-24.279	1.00 26.23
BBBBATOM	4461	CA	ALA	B	249	5.512	-22.216	-25.290	1.00 24.67
BBBBATOM	4462	CB	ALA	B	249	4.625	-22.069	-26.537	1.00 25.39
BBBBATOM	4463	C	ALA	B	249	5.870	-20.843	-24.721	1.00 24.03
BBBBATOM	4464	O	ALA	B	249	6.971	-20.338	-24.932	1.00 23.78
BBBBATOM	4465	N	ALA	B	250	4.942	-20.241	-23.983	1.00 23.39
BBBBATOM	4466	CA	ALA	B	250	5.188	-18.933	-23.390	1.00 21.78
BBBBATOM	4467	CB	ALA	B	250	3.898	-18.376	-22.797	1.00 23.21
BBBBATOM	4468	C	ALA	B	250	6.277	-19.011	-22.313	1.00 21.84
BBBBATOM	4469	O	ALA	B	250	7.091	-18.092	-22.176	1.00 20.78
BBBBATOM	4470	.N ,	ALA	B	251	6.291	-20.099	-21.548	1.00 20.34
BBBBATOM	4471	CA	ALA	B	251	7.301	-20.259	-20.501	1.00 20.85
BBBBATOM	4472	CB	ALA	B	251	6.920	-21.405	-19.568	1.00 19.79
BBBBATOM	4473	C	ALA	B	251	8.685	-20.512	-21.123	1.00 20.95
BBBBATOM	4474	O	ALA	B	251	9.689	-19.980	-20.648	1.00 21.14
BBBBATOM	4475	N	TYR	B	252	8.723	-21.314	-22.184	1.00 21.27
BBBBATOM	4476	CA	TYR	B	252	9.972	-21.616	-22.886	1.00 22.78
BBBBATOM	4477	CB	TYR	B	252	9.726	-22.661	-23.980	1.00 21.62
BBBBATOM	4478	CG	TYR	B	252	9.662	-24.100	-23.505	1.00 23.34
BBBBATOM	4479	CD1	TYR	B	252	9.003	-25.065	-24.261	1.00 22.88
BBBBATOM	4480	CE1	TYR	B	252	8.961	-26.392	-23.861	1.00 24.81
BBBBATOM	4481	CD2	TYR	B	252	10.288	-24.505	-22.319	1.00 22.30
BBBBATOM	4482	CE2	TYR	B	252	10.253	-25.838	-21.912	1.00 23.56
BBBBATOM	4483	CZ	TYR	B	252	9.590	-26.772	-22.687	1.00 24.26
BBBBATOM	4484	OH	TYR	B	252	9.554	-28.088	-22.305	1.00 25.57
BBBBATOM	4485	C	TYR	B	252	10.566	-20.354	-23.516	1.00 23.57
BBBBATOM	4486	O	TYR	B	252	11.784	-20.180	-23.550	1.00 23.91
BBBBATOM	4487	N	ALA	B	253	9.699	-19.473	-24.007	1.00 23.22
BBBBATOM	4488	CA	ALA	B	253	10.131	-18.224	-24.636	1.00 23.54
BBBBATOM	4489	CB	ALA	B	253	8.931	-17.512	-25.275	1.00 24.59
BBBBATOM	4490	C	ALA	B	253	10.783	-17.305	-23.617	1.00 23.30
BBBBATOM	4491	O	ALA	B	253	11.699	-16.546	-23.945	1.00 23.04
BBBBATOM	4492	N	TRP	B	254	10.299	-17.369	-22.379	1.00 20.49
BBBBATOM	4493	CA	TRP	B	254	10.829	-16.534	-21.303	1.00 19.76
BBBBATOM	4494	CB	TRP	B	254	9.808	-16.467	-20.151	1.00 19.57
BBBBATOM	4495	CG	TRP	B	254	10.381	-15.981	-18.841	1.00 19.57
BBBBATOM	4496	CD2	TRP	B	254	10.870	-16.796	-17.762	1.00 19.25
BBBBATOM	4497	CE2	TRP	B	254	11.369	-15.922	-16.771	1.00 18.94
BBBBATOM	4498	CE3	TRP	B	254	10.939	-18.178	-17.543	1.00 19.18
BBBBATOM	4499	CD1	TRP	B	254	10.591	-14.691	-18.470	1.00 19.03
BBBBATOM	4500	NE1	TRP	B	254	11.185	-14.643	-17.226	1.00 20.30
BBBBATOM	4501	CZ2	TRP	B	254	11.931	-16.382	-15.572	1.00 20.01
BBBBATOM	4502	CZ3	TRP	B	254	11.504	-18.642	-16.346	1.00 20.05
BBBBATOM	4503	CH2	TRP	B	254	11.991	-17.743	-15.380	1.00 18.31
BBBBATOM	4504	C	TRP	B	254	12.156	-17.059	-20.755	1.00 19.33
BBBBATOM	4505	O	TRP	B	254	13.084	-16.293	-20.496	1.00 19.25
BBBBATOM	4506	N	ALA	B	255	12.234	-18.373	-20.597	1.00 18.90
BBBBATOM	4507	CA	ALA	B	255	13.399	-19.025	-20.003	1.00 19.51
BBBBATOM	4508	CB	ALA	B	255	13.082	-20.507	-19.788	1.00 18.83
BBBBATOM	4509	C	ALA	B	255	14.737	-18.901	-20.713	1.00 18.88
BBBBATOM	4510	O	ALA	B	255	14.803	-18.688	-21.918	1.00 19.40
BBBBATOM	4511	N	ASP	B	256	15.803	-19.036	-19.927	1.00 19.01
BBBBATOM	4512	CA	ASP	B	256	17.176	-19.026	-20.434	1.00 17.58
BBBBATOM	4513	CB	ASP	B	256	18.078	-18.185	-19.534	1.00 18.47
BBBBATOM	4514	CG	ASP	B	256	17.954	-16.699	-19.795	1.00 18.05

BBBBATOM	4515	OD1	ASP	B	256	17.845	-15.944	-18.806	1.00	16.89
BBBBATOM	4516	OD2	ASP	B	256	17.983	-16.287	-20.982	1.00	19.53
BBBBATOM	4517	C	ASP	B	256	17.657	-20.481	-20.379	1.00	18.01
BBBBATOM	4518	O	ASP	B	256	18.459	-20.929	-21.198	1.00	16.11
BBBBATOM	4519	N	VAL	B	257	17.147	-21.216	-19.396	1.00	17.49
BBBBATOM	4520	CA	VAL	B	257	17.535	-22.603	-19.194	1.00	18.53
BBBBATOM	4521	CB	VAL	B	257	18.831	-22.681	-18.332	1.00	17.72
BBBBATOM	4522	CG1	VAL	B	257	18.586	-22.069	-16.966	1.00	19.19
BBBBATOM	4523	CG2	VAL	B	257	19.286	-24.129	-18.200	1.00	20.40
BBBBATOM	4524	C	VAL	B	257	16.400	-23.363	-18.501	1.00	18.31
BBBBATOM	4525	O	VAL	B	257	15.659	-22.795	-17.703	1.00	19.74
BBBBATOM	4526	N	VAL	B	258	16.263	-24.643	-18.818	1.00	18.74
BBBBATOM	4527	CA	VAL	B	258	15.208	-25.456	-18.234	1.00	19.32
BBBBATOM	4528	CB	VAL	B	258	14.328	-26.100	-19.337	1.00	19.89
BBBBATOM	4529	CG1	VAL	B	258	13.101	-26.754	-18.714	1.00	19.81
BBBBATOM	4530	CG2	VAL	B	258	13.907	-25.041	-20.364	1.00	21.59
BBBBATOM	4531	C	VAL	B	258	15.799	-26.585	-17.389	1.00	19.70
BBBBATOM	4532	O	VAL	B	258	16.808	-27.175	-17.758	1.00	18.96
BBBBATOM	4533	N	VAL	B	259	15.167	-26.861	-16.253	1.00	20.24
BBBBATOM	4534	CA	VAL	B	259	15.581	-27.957	-15.374	1.00	19.85
BBBBATOM	4535	CB	VAL	B	259	15.850	-27.483	-13.936	1.00	20.08
BBBBATOM	4536	.CG1	VAL	B	259	16.222	-28.689	-13.059	1.00	20.22
BBBBATOM	4537	CG2	VAL	B	259	16.966	-26.453	-13.930	1.00	17.86
BBBBATOM	4538	C	VAL	B	259	14.382	-28.890	-15.371	1.00	20.02
BBBBATOM	4539	O	VAL	B	259	13.301	-28.500	-14.942	1.00	21.88
BBBBATOM	4540	N	CYS	B	260	14.562	-30.111	-15.867	1.00	21.70
BBBBATOM	4541	CA	CYS	B	260	13.454	-31.055	-15.946	1.00	22.00
BBBBATOM	4542	CB	CYS	B	260	12.494	-30.618	-17.057	1.00	22.77
BBBBATOM	4543	SG	CYS	B	260	13.297	-30.506	-18.711	1.00	22.15
BBBBATOM	4544	C	CYS	B	260	13.903	-32.478	-16.242	1.00	21.86
BBBBATOM	4545	O	CYS	B	260	15.087	-32.730	-16.496	1.00	21.34
BBBBATOM	4546	N	ARG	B	261	12.937	-33.397	-16.212	1.00	22.34
BBBBATOM	4547	CA	ARG	B	261	13.170	-34.800	-16.515	1.00	23.75
BBBBATOM	4548	CB	ARG	B	261	11.964	-35.663	-16.104	1.00	27.16
BBBBATOM	4549	CG	ARG	B	261	11.376	-35.337	-14.738	1.00	31.82
BBBBATOM	4550	CD	ARG	B	261	11.490	-36.473	-13.732	1.00	36.33
BBBBATOM	4551	NE	ARG	B	261	12.865	-36.721	-13.323	1.00	38.48
BBBBATOM	4552	CZ	ARG	B	261	13.218	-37.176	-12.125	1.00	37.25
BBBBATOM	4553	NH1	ARG	B	261	12.295	-37.433	-11.204	1.00	38.46
BBBBATOM	4554	NH2	ARG	B	261	14.499	-37.370	-11.848	1.00	36.79
BBBBATOM	4555	C	ARG	B	261	13.351	-34.871	-18.032	1.00	23.98
BBBBATOM	4556	O	ARG	B	261	13.117	-33.883	-18.746	1.00	22.44
BBBBATOM	4557	N	SER	B	262	13.740	-36.038	-18.527	1.00	22.00
BBBBATOM	4558	CA	SER	B	262	13.975	-36.189	-19.948	1.00	23.18
BBBBATOM	4559	CB	SER	B	262	15.481	-36.377	-20.203	1.00	24.45
BBBBATOM	4560	OG	SER	B	262	16.043	-37.326	-19.311	1.00	25.79
BBBBATOM	4561	C	SER	B	262	13.173	-37.263	-20.676	1.00	22.90
BBBBATOM	4562	O	SER	B	262	13.738	-38.179	-21.274	1.00	23.25
BBBBATOM	4563	N	GLY	B	263	11.850	-37.151	-20.619	1.00	22.74
BBBBATOM	4564	CA	GLY	B	263	11.026	-38.079	-21.361	1.00	22.85
BBBBATOM	4565	C	GLY	B	263	11.392	-37.793	-22.813	1.00	24.06
BBBBATOM	4566	O	GLY	B	263	11.908	-36.705	-23.121	1.00	22.75
BBBBATOM	4567	N	ALA	B	264	11.130	-38.739	-23.708	1.00	23.37
BBBBATOM	4568	CA	ALA	B	264	11.482	-38.564	-25.115	1.00	24.25
BBBBATOM	4569	CB	ALA	B	264	11.133	-39.829	-25.894	1.00	24.58
BBBBATOM	4570	C	ALA	B	264	10.843	-37.343	-25.783	1.00	24.29
BBBBATOM	4571	O	ALA	B	264	11.523	-36.572	-26.470	1.00	24.33
BBBBATOM	4572	N	LEU	B	265	9.541	-37.167	-25.596	1.00	24.44
BBBBATOM	4573	CA	LEU	B	265	8.846	-36.037	-26.205	1.00	24.66
BBBBATOM	4574	CB	LEU	B	265	7.332	-36.183	-26.011	1.00	25.33
BBBBATOM	4575	CG	LEU	B	265	6.760	-37.544	-26.426	1.00	27.97
BBBBATOM	4576	CD1	LEU	B	265	5.242	-37.541	-26.258	1.00	28.21
BBBBATOM	4577	CD2	LEU	B	265	7.146	-37.856	-27.878	1.00	27.40
BBBBATOM	4578	C	LEU	B	265	9.331	-34.717	-25.613	1.00	24.47
BBBBATOM	4579	O	LEU	B	265	9.374	-33.693	-26.301	1.00	23.85
BBBBATOM	4580	N	THR	B	266	9.702	-34.747	-24.338	1.00	22.12

BBBBATOM	4581	CA	THR	B	266	10.194	-33.557	-23.657	1.00	22.34
BBBBATOM	4582	CB	THR	B	266	10.348	-33.803	-22.140	1.00	22.35
BBBBATOM	4583	OG1	THR	B	266	9.061	-34.087	-21.583	1.00	24.46
BBBBATOM	4584	CG2	THR	B	266	10.945	-32.573	-21.444	1.00	24.00
BBBBATOM	4585	C	THR	B	266	11.535	-33.117	-24.226	1.00	21.15
BBBBATOM	4586	O	THR	B	266	11.761	-31.926	-24.442	1.00	20.35
BBBBATOM	4587	N	VAL	B	267	12.427	-34.075	-24.461	1.00	20.46
BBBBATOM	4588	CA	VAL	B	267	13.730	-33.762	-25.023	1.00	21.11
BBBBATOM	4589	CB	VAL	B	267	14.614	-35.039	-25.114	1.00	21.54
BBBBATOM	4590	CG1	VAL	B	267	15.903	-34.740	-25.865	1.00	20.72
BBBBATOM	4591	CG2	VAL	B	267	14.938	-35.541	-23.708	1.00	20.45
BBBBATOM	4592	C	VAL	B	267	13.548	-33.138	-26.416	1.00	21.34
BBBBATOM	4593	O	VAL	B	267	14.188	-32.135	-26.747	1.00	19.99
BBBBATOM	4594	N	SER	B	268	12.663	-33.717	-27.222	1.00	21.61
BBBBATOM	4595	CA	SER	B	268	12.411	-33.191	-28.567	1.00	21.96
BBBBATOM	4596	CB	SER	B	268	11.474	-34.121	-29.344	1.00	21.57
BBBBATOM	4597	OG	SER	B	268	12.141	-35.316	-29.721	1.00	24.06
BBBBATOM	4598	C	SER	B	268	11.817	-31.790	-28.519	1.00	21.81
BBBBATOM	4599	O	SER	B	268	12.158	-30.933	-29.336	1.00	22.60
BBBBATOM	4600	N	GLU	B	269	10.928	-31.563	-27.557	1.00	21.64
BBBBATOM	4601	CA	GLU	B	269	10.282	-30.272	-27.378	1.00	21.95
BBBBATOM	4602	CB	GLU	B	269	9.213	-30.399	-26.292	1.00	24.72
BBBBATOM	4603	CG	GLU	B	269	8.480	-29.128	-25.940	1.00	27.67
BBBBATOM	4604	CD	GLU	B	269	7.385	-29.380	-24.908	1.00	30.05
BBBBATOM	4605	OE1	GLU	B	269	6.325	-29.915	-25.287	1.00	31.50
BBBBATOM	4606	OE2	GLU	B	269	7.591	-29.057	-23.719	1.00	29.84
BBBBATOM	4607	C	GLU	B	269	11.321	-29.214	-26.999	1.00	21.68
BBBBATOM	4608	O	GLU	B	269	11.301	-28.095	-27.518	1.00	18.12
BBBBATOM	4609	N	ILE	B	270	12.224	-29.581	-26.092	1.00	19.43
BBBBATOM	4610	CA	ILE	B	270	13.295	-28.698	-25.638	1.00	20.62
BBBBATOM	4611	CB	ILE	B	270	14.157	-29.391	-24.533	1.00	20.30
BBBBATOM	4612	CG2	ILE	B	270	15.415	-28.595	-24.266	1.00	19.17
BBBBATOM	4613	CG1	ILE	B	270	13.337	-29.574	-23.254	1.00	21.32
BBBBATOM	4614	CD1	ILE	B	270	12.926	-28.291	-22.583	1.00	23.40
BBBBATOM	4615	C	ILE	B	270	14.214	-28.314	-26.806	1.00	20.58
BBBBATOM	4616	O	ILE	B	270	14.595	-27.151	-26.954	1.00	20.50
BBBBATOM	4617	N	ALA	B	271	14.574	-29.298	-27.624	1.00	21.29
BBBBATOM	4618	CA	ALA	B	271	15.440	-29.058	-28.776	1.00	22.45
BBBBATOM	4619	CB	ALA	B	271	15.741	-30.376	-29.485	1.00	23.36
BBBBATOM	4620	C	ALA	B	271	14.766	-28.084	-29.745	1.00	23.03
BBBBATOM	4621	O	ALA	B	271	15.400	-27.156	-30.259	1.00	23.57
BBBBATOM	4622	N	ALA	B	272	13.479	-28.301	-29.988	1.00	21.81
BBBBATOM	4623	CA	ALA	B	272	12.719	-27.451	-30.898	1.00	22.17
BBBBATOM	4624	CB	ALA	B	272	11.335	-28.053	-31.131	1.00	22.15
BBBBATOM	4625	C	ALA	B	272	12.590	-26.030	-30.355	1.00	22.78
BBBBATOM	4626	O	ALA	B	272	12.585	-25.058	-31.122	1.00	21.77
BBBBATOM	4627	N	ALA	B	273	12.474	-25.907	-29.034	1.00	21.06
BBBBATOM	4628	CA	ALA	B	273	12.361	-24.596	-28.407	1.00	21.97
BBBBATOM	4629	CB	ALA	B	273	11.919	-24.737	-26.949	1.00	20.63
BBBBATOM	4630	C	ALA	B	273	13.699	-23.867	-28.468	1.00	21.83
BBBBATOM	4631	O	ALA	B	273	13.754	-22.642	-28.344	1.00	22.67
BBBBATOM	4632	N	GLY	B	274	14.773	-24.621	-28.656	1.00	20.90
BBBBATOM	4633	CA	GLY	B	274	16.093	-24.023	-28.709	1.00	21.07
BBBBATOM	4634	C	GLY	B	274	16.498	-23.549	-27.327	1.00	21.48
BBBBATOM	4635	O	GLY	B	274	16.961	-22.421	-27.154	1.00	20.01
BBBBATOM	4636	N	LEU	B	275	16.331	-24.420	-26.333	1.00	19.66
BBBBATOM	4637	CA	LEU	B	275	16.666	-24.057	-24.966	1.00	19.78
BBBBATOM	4638	CB	LEU	B	275	15.402	-24.068	-24.102	1.00	21.30
BBBBATOM	4639	CG	LEU	B	275	14.451	-22.870	-24.202	1.00	24.60
BBBBATOM	4640	CD1	LEU	B	275	13.220	-23.136	-23.349	1.00	26.44
BBBBATOM	4641	CD2	LEU	B	275	15.159	-21.609	-23.725	1.00	24.02
BBBBATOM	4642	C	LEU	B	275	17.698	-24.970	-24.318	1.00	18.79
BBBBATOM	4643	O	LEU	B	275	17.679	-26.180	-24.524	1.00	19.36
BBBBATOM	4644	N	PRO	B	276	18.634	-24.389	-23.554	1.00	17.27
BBBBATOM	4645	CD	PRO	B	276	18.925	-22.955	-23.416	1.00	16.95
BBBBATOM	4646	CA	PRO	B	276	19.651	-25.199	-22.875	1.00	16.62

BBBBATOM	4647	CB	PRO	B	276	20.619	-24.162	-22.317	1.00	17.27
BBBBATOM	4648	CG	PRO	B	276	20.408	-22.957	-23.195	1.00	18.59
BBBBATOM	4649	C	PRO	B	276	18.900	-25.900	-21.746	1.00	17.23
BBBBATOM	4650	O	PRO	B	276	17.944	-25.340	-21.189	1.00	15.14
BBBBATOM	4651	N	ALA	B	277	19.316	-27.110	-21.396	1.00	17.01
BBBBATOM	4652	CA	ALA	B	277	18.638	-27.807	-20.321	1.00	15.80
BBBBATOM	4653	CB	ALA	B	277	17.641	-28.805	-20.895	1.00	17.01
BBBBATOM	4654	C	ALA	B	277	19.591	-28.526	-19.382	1.00	17.37
BBBBATOM	4655	O	ALA	B	277	20.710	-28.891	-19.755	1.00	17.09
BBBBATOM	4656	N	LEU	B	278	19.147	-28.673	-18.138	1.00	17.14
BBBBATOM	4657	CA	LEU	B	278	19.896	-29.429	-17.145	1.00	18.48
BBBBATOM	4658	CB	LEU	B	278	20.140	-28.619	-15.869	1.00	19.19
BBBBATOM	4659	CG	LEU	B	278	21.084	-29.308	-14.868	1.00	20.85
BBBBATOM	4660	CD1	LEU	B	278	21.283	-28.411	-13.668	1.00	21.11
BBBBATOM	4661	CD2	LEU	B	278	20.497	-30.647	-14.433	1.00	19.16
BBBBATOM	4662	C	LEU	B	278	18.884	-30.535	-16.898	1.00	19.62
BBBBATOM	4663	O	LEU	B	278	17.870	-30.330	-16.218	1.00	20.77
BBBBATOM	4664	N	PHE	B	279	19.149	-31.691	-17.495	1.00	19.50
BBBBATOM	4665	CA	PHE	B	279	18.266	-32.838	-17.392	1.00	21.59
BBBBATOM	4666	CB	PHE	B	279	18.385	-33.700	-18.651	1.00	21.07
BBBBATOM	4667	CG	PHE	B	279	17.740	-33.099	-19.876	1.00	19.35
BBBBATOM	4668	CD1	PHE	B	279	18.481	-32.898	-21.035	1.00	19.42
BBBBATOM	4669	CD2	PHE	B	279	16.379	-32.794	-19.888	1.00	18.16
BBBBATOM	4670	CE1	PHE	B	279	17.874	-32.405	-22.203	1.00	19.06
BBBBATOM	4671	CE2	PHE	B	279	15.759	-32.298	-21.052	1.00	17.65
BBBBATOM	4672	CZ	PHE	B	279	16.515	-32.108	-22.208	1.00	15.61
BBBBATOM	4673	C	PHE	B	279	18.525	-33.709	-16.167	1.00	22.86
BBBBATOM	4674	O	PHE	B	279	19.671	-34.065	-15.871	1.00	23.32
BBBBATOM	4675	N	VAL	B	280	17.445	-34.037	-15.461	1.00	23.88
BBBBATOM	4676	CA	VAL	B	280	17.502	-34.902	-14.281	1.00	25.67
BBBBATOM	4677	CB	VAL	B	280	16.883	-34.223	-13.048	1.00	26.89
BBBBATOM	4678	CG1	VAL	B	280	16.954	-35.159	-11.847	1.00	28.12
BBBBATOM	4679	CG2	VAL	B	280	17.631	-32.929	-12.742	1.00	27.70
BBBBATOM	4680	C	VAL	B	280	16.690	-36.136	-14.658	1.00	25.65
BBBBATOM	4681	O	VAL	B	280	15.509	-36.239	-14.346	1.00	24.57
BBBBATOM	4682	N	PRO	B	281	17.324	-37.080	-15.370	1.00	27.08
BBBBATOM	4683	CD	PRO	B	281	18.750	-37.057	-15.726	1.00	27.31
BBBBATOM	4684	CA	PRO	B	281	16.698	-38.320	-15.824	1.00	29.05
BBBBATOM	4685	CB	PRO	B	281	17.851	-39.071	-16.492	1.00	29.44
BBBBATOM	4686	CG	PRO	B	281	18.791	-37.992	-16.895	1.00	29.67
BBBBATOM	4687	C	PRO	B	281	16.092	-39.121	-14.684	1.00	31.51
BBBBATOM	4688	O	PRO	B	281	16.675	-39.223	-13.603	1.00	32.26
BBBBATOM	4689	N	PHE	B	282	14.908	-39.668	-14.923	1.00	33.83
BBBBATOM	4690	CA	PHE	B	282	14.246	-40.496	-13.926	1.00	37.13
BBBBATOM	4691	CB	PHE	B	282	12.818	-40.808	-14.372	1.00	38.38
BBBBATOM	4692	CG	PHE	B	282	12.032	-41.606	-13.377	1.00	40.57
BBBBATOM	4693	CD1	PHE	B	282	11.720	-41.074	-12.130	1.00	41.80
BBBBATOM	4694	CD2	PHE	B	282	11.590	-42.886	-13.689	1.00	41.65
BBBBATOM	4695	CE1	PHE	B	282	10.975	-41.806	-11.209	1.00	42.03
BBBBATOM	4696	CE2	PHE	B	282	10.843	-43.628	-12.773	1.00	42.49
BBBBATOM	4697	CZ	PHE	B	282	10.536	-43.085	-11.532	1.00	41.74
BBBBATOM	4698	C	PHE	B	282	15.078	-41.776	-13.880	1.00	38.09
BBBBATOM	4699	O	PHE	B	282	15.357	-42.373	-14.921	1.00	38.33
BBBBATOM	4700	N	GLN	B	283	15.492	-42.197	-12.690	1.00	39.70
BBBBATOM	4701	CA	GLN	B	283	16.319	-43.395	-12.591	1.00	41.11
BBBBATOM	4702	CB	GLN	B	283	17.010	-43.477	-11.223	1.00	41.41
BBBBATOM	4703	CG	GLN	B	283	17.953	-44.676	-11.096	1.00	42.60
BBBBATOM	4704	CD	GLN	B	283	19.143	-44.605	-12.051	1.00	42.87
BBBBATOM	4705	OE1	GLN	B	283	20.199	-44.068	-11.712	1.00	43.66
BBBBATOM	4706	NE2	GLN	B	283	18.969	-45.135	-13.254	1.00	42.46
BBBBATOM	4707	C	GLN	B	283	15.543	-44.679	-12.846	1.00	41.60
BBBBATOM	4708	O	GLN	B	283	14.382	-44.809	-12.462	1.00	40.91
BBBBATOM	4709	N	HIS	B	284	16.211	-45.618	-13.511	1.00	42.92
BBBBATOM	4710	CA	HIS	B	284	15.641	-46.917	-13.843	1.00	43.69
BBBBATOM	4711	CB	HIS	B	284	14.508	-46.760	-14.858	1.00	43.91
BBBBATOM	4712	CG	HIS	B	284	13.795	-48.039	-15.165	1.00	44.71

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BBBBATOM	4713	CD2	HIS	B	284	12.574	-48.489	-14.793	1.00 44.80
BBBBATOM	4714	ND1	HIS	B	284	14.360	-49.044	-15.923	1.00 44.69
BBBBATOM	4715	CE1	HIS	B	284	13.516	-50.058	-16.002	1.00 45.06
BBBBATOM	4716	NE2	HIS	B	284	12.425	-49.747	-15.325	1.00 44.90
BBBBATOM	4717	C	HIS	B	284	16.749	-47.788	-14.424	1.00 44.09
BBBBATOM	4718	O	HIS	B	284	17.602	-47.302	-15.164	1.00 43.02
BBBBATOM	4719	N	LYS	B	285	16.740	-49.074	-14.085	1.00 44.90
BBBBATOM	4720	CA	LYS	B	285	17.767	-49.993	-14.571	1.00 45.34
BBBBATOM	4721	CB	LYS	B	285	17.386	-51.436	-14.222	1.00 46.84
BBBBATOM	4722	CG	LYS	B	285	18.541	-52.425	-14.327	1.00 49.53
BBBBATOM	4723	CD	LYS	B	285	18.140	-53.802	-13.807	1.00 51.08
BBBBATOM	4724	CE	LYS	B	285	19.325	-54.759	-13.780	1.00 51.58
BBBBATOM	4725	NZ	LYS	B	285	18.931	-56.115	-13.292	1.00 52.11
BBBBATOM	4726	C	LYS	B	285	17.969	-49.853	-16.079	1.00 45.02
BBBBATOM	4727	O	LYS	B	285	19.067	-50.070	-16.595	1.00 45.49
BBBBATOM	4728	N	ASP	B	286	16.903	-49.478	-16.777	1.00 44.33
BBBBATOM	4729	CA	ASP	B	286	16.949	-49.299	-18.222	1.00 43.26
BBBBATOM	4730	CB	ASP	B	286	15.532	-49.379	-18.794	1.00 45.91
BBBBATOM	4731	CG	ASP	B	286	15.511	-49.354	-20.304	1.00 48.32
BBBBATOM	4732	OD1	ASP	B	286	15.971	-50.338	-20.925	1.00 49.52
BBBBATOM	4733	OD2	ASP	B	286	15.037	-48.346	-20.872	1.00 51.04
BBBBATOM	4734	.C ,	ASP	B	286	17.573	-47.947	-18.582	1.00 40.92
BBBBATOM	4735	O'	ASP	B	286	18.179	-47.796	-19.643	1.00 40.31
BBBBATOM	4736	N	ARG	B	287	17.415	-46.972	-17.689	1.00 38.60
BBBBATOM	4737	CA	ARG	B	287	17.951	-45.623	-17.883	1.00 36.28
BBBBATOM	4738	CB	ARG	B	287	19.477	-45.650	-17.910	1.00 37.28
BBBBATOM	4739	CG	ARG	B	287	20.116	-46.263	-16.687	1.00 40.54
BBBBATOM	4740	CD	ARG	B	287	21.605	-46.395	-16.906	1.00 42.34
BBBBATOM	4741	NE	ARG	B	287	22.291	-45.113	-16.802	1.00 44.33
BBBBATOM	4742	CZ	ARG	B	287	23.449	-44.842	-17.392	1.00 45.20
BBBBATOM	4743	NH1	ARG	B	287	24.045	-45.764	-18.135	1.00 45.60
BBBBATOM	4744	NH2	ARG	B	287	24.019	-43.656	-17.227	1.00 45.68
BBBBATOM	4745	C	ARG	B	287	17.449	-45.005	-19.180	1.00 33.59
BBBBATOM	4746	O	ARG	B	287	18.167	-44.255	-19.844	1.00 32.61
BBBBATOM	4747	N	GLN	B	288	16.212	-45.321	-19.533	1.00 30.94
BBBBATOM	4748	CA	GLN	B	288	15.622	-44.804	-20.755	1.00 30.77
BBBBATOM	4749	CB	GLN	B	288	14.143	-45.158	-20.810	1.00 30.59
BBBBATOM	4750	CG	GLN	B	288	13.473	-44.772	-22.109	1.00 29.73
BBBBATOM	4751	CD	GLN	B	288	11.981	-44.971	-22.044	1.00 28.04
BBBBATOM	4752	OE1	GLN	B	288	11.294	-44.295	-21.279	1.00 29.59
BBBBATOM	4753	NE2	GLN	B	288	11.468	-45.905	-22.838	1.00 26.98
BBBBATOM	4754	C	GLN	B	288	15.783	-43.291	-20.885	1.00 29.70
BBBBATOM	4755	O	GLN	B	288	16.268	-42.801	-21.902	1.00 29.79
BBBBATOM	4756	N	GLN	B	289	15.378	-42.554	-19.857	1.00 29.38
BBBBATOM	4757	CA	GLN	B	289	15.474	-41.099	-19.904	1.00 29.46
BBBBATOM	4758	CB	GLN	B	289	14.772	-40.472	-18.700	1.00 29.25
BBBBATOM	4759	CG	GLN	B	289	13.265	-40.416	-18.883	1.00 29.32
BBBBATOM	4760	CD	GLN	B	289	12.575	-39.585	-17.826	1.00 29.84
BBBBATOM	4761	OE1	GLN	B	289	13.191	-38.728	-17.188	1.00 29.52
BBBBATOM	4762	NE2	GLN	B	289	11.281	-39.821	-17.647	1.00 28.95
BBBBATOM	4763	C	GLN	B	289	16.906	-40.613	-20.005	1.00 29.36
BBBBATOM	4764	O	GLN	B	289	17.173	-39.557	-20.585	1.00 29.12
BBBBATOM	4765	N	TYR	B	290	17.835	-41.374	-19.442	1.00 28.95
BBBBATOM	4766	CA	TYR	B	290	19.228	-40.984	-19.550	1.00 29.55
BBBBATOM	4767	CB	TYR	B	290	20.136	-41.934	-18.768	1.00 31.40
BBBBATOM	4768	CG	TYR	B	290	21.587	-41.780	-19.148	1.00 33.37
BBBBATOM	4769	CD1	TYR	B	290	22.332	-40.682	-18.717	1.00 34.57
BBBBATOM	4770	CE1	TYR	B	290	23.644	-40.490	-19.148	1.00 35.97
BBBBATOM	4771	CD2	TYR	B	290	22.192	-42.684	-20.017	1.00 34.90
BBBBATOM	4772	CE2	TYR	B	290	23.497	-42.500	-20.453	1.00 36.03
BBBBATOM	4773	CZ	TYR	B	290	24.214	-41.402	-20.019	1.00 36.29
BBBBATOM	4774	OH	TYR	B	290	25.499	-41.215	-20.475	1.00 39.44
BBBBATOM	4775	C	TYR	B	290	19.593	-41.042	-21.032	1.00 28.80
BBBBATOM	4776	O	TYR	B	290	20.192	-40.113	-21.567	1.00 29.22
BBBBATOM	4777	N	TRP	B	291	19.227	-42.135	-21.697	1.00 27.57
BBBBATOM	4778	CA	TRP	B	291	19.542	-42.282	-23.116	1.00 28.07

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BBBBATOM   4779   CB    TRP  B  291      19.217  -43.705  -23.599   1.00  29.42
BBBBATOM   4780   CG    TRP  B  291      20.070  -44.750  -22.936   1.00  31.82
BBBBATOM   4781   CD2   TRP  B  291      21.487  -44.908  -23.069   1.00  33.22
BBBBATOM   4782   CE2   TRP  B  291      21.873  -45.966  -22.213   1.00  33.81
BBBBATOM   4783   CE3   TRP  B  291      22.470  -44.257  -23.826   1.00  33.13
BBBBATOM   4784   CD1   TRP  B  291      19.663  -45.695  -22.035   1.00  32.62
BBBBATOM   4785   NE1   TRP  B  291      20.741  -46.428  -21.595   1.00  33.43
BBBBATOM   4786   CZ2   TRP  B  291      23.203  -46.387  -22.093   1.00  34.69
BBBBATOM   4787   CZ3   TRP  B  291      23.794  -44.676  -23.707   1.00  35.41
BBBBATOM   4788   CH2   TRP  B  291      24.146  -45.732  -22.845   1.00  35.26
BBBBATOM   4789   C     TRP  B  291      18.808  -41.256  -23.978   1.00  26.84
BBBBATOM   4790   O     TRP  B  291      19.283  -40.900  -25.058   1.00  26.55
BBBBATOM   4791   N     ASN  B  292      17.658  -40.779  -23.508   1.00  25.52
BBBBATOM   4792   CA    ASN  B  292      16.902  -39.784  -24.270   1.00  26.06
BBBBATOM   4793   CB    ASN  B  292      15.484  -39.599  -23.709   1.00  24.78
BBBBATOM   4794   CG    ASN  B  292      14.590  -40.811  -23.928   1.00  24.46
BBBBATOM   4795   OD1   ASN  B  292      14.842  -41.641  -24.798   1.00  25.33
BBBBATOM   4796   ND2   ASN  B  292      13.523  -40.900  -23.146   1.00  23.83
BBBBATOM   4797   C     ASN  B  292      17.605  -38.427  -24.258   1.00  25.99
BBBBATOM   4798   O     ASN  B  292      17.566  -37.687  -25.244   1.00  26.18
BBBBATOM   4799   N     ALA  B  293      18.242  -38.105  -23.139   1.00  25.66
BBBBATOM   4800   .CA   ALA  B  293      18.926  -36.822  -22.979   1.00  25.69
BBBBATOM   4801   CB    ALA  B  293      18.940  -36.422  -21.506   1.00  24.17
BBBBATOM   4802   C     ALA  B  293      20.346  -36.800  -23.521   1.00  25.67
BBBBATOM   4803   O     ALA  B  293      20.855  -35.743  -23.902   1.00  25.52
BBBBATOM   4804   N     LEU  B  294      20.978  -37.969  -23.560   1.00  25.62
BBBBATOM   4805   CA    LEU  B  294      22.354  -38.088  -24.032   1.00  25.90
BBBBATOM   4806   CB    LEU  B  294      22.745  -39.566  -24.121   1.00  26.51
BBBBATOM   4807   CG    LEU  B  294      24.226  -39.864  -24.350   1.00  28.12
BBBBATOM   4808   CD1   LEU  B  294      25.085  -39.055  -23.380   1.00  28.29
BBBBATOM   4809   CD2   LEU  B  294      24.470  -41.368  -24.169   1.00  28.15
BBBBATOM   4810   C     LEU  B  294      22.644  -37.392  -25.359   1.00  25.66
BBBBATOM   4811   O     LEU  B  294      23.677  -36.741  -25.507   1.00  24.79
BBBBATOM   4812   N     PRO  B  295      21.748  -37.532  -26.351   1.00  26.24
BBBBATOM   4813   CD    PRO  B  295      20.560  -38.400  -26.437   1.00  25.75
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BBBBATOM   4815   CB    PRO  B  295      20.740  -37.201  -28.439   1.00  26.70
BBBBATOM   4816   CG    PRO  B  295      20.382  -38.548  -27.932   1.00  26.84
BBBBATOM   4817   C     PRO  B  295      22.219  -35.358  -27.480   1.00  25.78
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BBBBATOM   4819   N     LEU  B  296      21.375  -34.703  -26.688   1.00  25.66
BBBBATOM   4820   CA    LEU  B  296      21.521  -33.265  -26.481   1.00  25.42
BBBBATOM   4821   CB    LEU  B  296      20.283  -32.685  -25.779   1.00  24.45
BBBBATOM   4822   CG    LEU  B  296      19.066  -32.458  -26.679   1.00  25.59
BBBBATOM   4823   CD1   LEU  B  296      17.968  -31.718  -25.911   1.00  23.56
BBBBATOM   4824   CD2   LEU  B  296      19.496  -31.630  -27.893   1.00  25.87
BBBBATOM   4825   C     LEU  B  296      22.784  -32.935  -25.688   1.00  26.07
BBBBATOM   4826   O     LEU  B  296      23.435  -31.917  -25.944   1.00  25.26
BBBBATOM   4827   N     GLU  B  297      23.143  -33.785  -24.730   1.00  26.14
BBBBATOM   4828   CA    GLU  B  297      24.354  -33.530  -23.953   1.00  28.78
BBBBATOM   4829   CB    GLU  B  297      24.470  -34.483  -22.755   1.00  29.05
BBBBATOM   4830   CG    GLU  B  297      25.716  -34.210  -21.908   1.00  30.81
BBBBATOM   4831   CD    GLU  B  297      25.812  -35.087  -20.671   1.00  31.84
BBBBATOM   4832   OE1   GLU  B  297      25.655  -34.555  -19.551   1.00  31.74
BBBBATOM   4833   OE2   GLU  B  297      26.045  -36.307  -20.820   1.00  31.56
BBBBATOM   4834   C     GLU  B  297      25.577  -33.686  -24.846   1.00  29.06
BBBBATOM   4835   O     GLU  B  297      26.528  -32.910  -24.746   1.00  29.11
BBBBATOM   4836   N     LYS  B  298      25.543  -34.688  -25.722   1.00  31.21
BBBBATOM   4837   CA    LYS  B  298      26.644  -34.947  -26.648   1.00  31.90
BBBBATOM   4838   CB    LYS  B  298      26.379  -36.216  -27.464   1.00  33.65
BBBBATOM   4839   CG    LYS  B  298      26.519  -37.514  -26.680   1.00  36.05
BBBBATOM   4840   CD    LYS  B  298      26.251  -38.734  -27.568   1.00  37.69
BBBBATOM   4841   CE    LYS  B  298      26.461  -40.033  -26.801   1.00  38.51
BBBBATOM   4842   NZ    LYS  B  298      26.094  -41.235  -27.607   1.00  39.05
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BBBBATOM   4844   O     LYS  B  298      27.945  -33.455  -27.998   1.00  30.87
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BBBBATOM	4845	N	ALA	B	299	25.725	-33.116	-27.952	1.00	31.63
BBBBATOM	4846	CA	ALA	B	299	25.773	-31.965	-28.847	1.00	30.38
BBBBATOM	4847	CB	ALA	B	299	24.415	-31.778	-29.521	1.00	30.22
BBBBATOM	4848	C	ALA	B	299	26.173	-30.685	-28.106	1.00	29.94
BBBBATOM	4849	O	ALA	B	299	26.278	-29.615	-28.709	1.00	30.96
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BBBBATOM	4851	CA	GLY	B	300	26.777	-29.635	-26.017	1.00	26.18
BBBBATOM	4852	C	GLY	B	300	25.619	-28.665	-25.810	1.00	25.19
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BBBBATOM	4854	N	ALA	B	301	24.392	-29.179	-25.820	1.00	23.51
BBBBATOM	4855	CA	ALA	B	301	23.214	-28.333	-25.638	1.00	22.50
BBBBATOM	4856	CB	ALA	B	301	22.174	-28.644	-26.717	1.00	23.44
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BBBBATOM	4858	O	ALA	B	301	21.705	-27.746	-23.863	1.00	19.90
BBBBATOM	4859	N	ALA	B	302	23.066	-29.504	-23.507	1.00	20.94
BBBBATOM	4860	CA	ALA	B	302	22.516	-29.770	-22.186	1.00	21.78
BBBBATOM	4861	CB	ALA	B	302	21.243	-30.595	-22.327	1.00	20.10
BBBBATOM	4862	C	ALA	B	302	23.503	-30.507	-21.288	1.00	22.69
BBBBATOM	4863	O	ALA	B	302	24.561	-30.948	-21.739	1.00	22.25
BBBBATOM	4864	N	LYS	B	303	23.156	-30.613	-20.009	1.00	24.62
BBBBATOM	4865	CA	LYS	B	303	23.979	-31.340	-19.048	1.00	25.86
BBBBATOM	4866	CB	LYS	B	303	24.632	-30.401	-18.036	1.00	27.85
BBBBATOM	4867	CG	LYS	B	303	25.466	-31.146	-16.986	1.00	29.37
BBBBATOM	4868	CD	LYS	B	303	26.150	-30.186	-16.025	1.00	32.41
BBBBATOM	4869	CE	LYS	B	303	27.083	-30.912	-15.056	1.00	33.22
BBBBATOM	4870	NZ	LYS	B	303	27.827	-29.952	-14.181	1.00	33.62
BBBBATOM	4871	C	LYS	B	303	23.083	-32.319	-18.302	1.00	26.41
BBBBATOM	4872	O	LYS	B	303	22.015	-31.948	-17.802	1.00	25.76
BBBBATOM	4873	N	ILE	B	304	23.520	-33.570	-18.234	1.00	25.65
BBBBATOM	4874	CA	ILE	B	304	22.753	-34.598	-17.550	1.00	27.17
BBBBATOM	4875	CB	ILE	B	304	22.786	-35.946	-18.316	1.00	27.06
BBBBATOM	4876	CG2	ILE	B	304	21.977	-36.996	-17.555	1.00	28.49
BBBBATOM	4877	CG1	ILE	B	304	22.242	-35.769	-19.733	1.00	27.61
BBBBATOM	4878	CD1	ILE	B	304	22.380	-37.009	-20.599	1.00	27.05
BBBBATOM	4879	C	ILE	B	304	23.308	-34.855	-16.160	1.00	27.00
BBBBATOM	4880	O	ILE	B	304	24.511	-35.012	-15.986	1.00	27.46
BBBBATOM	4881	N	ILE	B	305	22.428	-34.869	-15.168	1.00	27.22
BBBBATOM	4882	CA	ILE	B	305	22.843	-35.178	-13.813	1.00	29.01
BBBBATOM	4883	CB	ILE	B	305	22.713	-33.977	-12.858	1.00	28.91
BBBBATOM	4884	CG2	ILE	B	305	23.063	-34.416	-11.432	1.00	30.98
BBBBATOM	4885	CG1	ILE	B	305	23.660	-32.855	-13.299	1.00	29.51
BBBBATOM	4886	CD1	ILE	B	305	23.674	-31.653	-12.367	1.00	29.43
BBBBATOM	4887	C	ILE	B	305	21.934	-36.302	-13.351	1.00	29.64
BBBBATOM	4888	O	ILE	B	305	20.806	-36.067	-12.932	1.00	29.25
BBBBATOM	4889	N	GLU	B	306	22.429	-37.532	-13.467	1.00	32.18
BBBBATOM	4890	CA	GLU	B	306	21.664	-38.702	-13.061	1.00	34.65
BBBBATOM	4891	CB	GLU	B	306	22.356	-39.989	-13.530	1.00	34.79
BBBBATOM	4892	CG	GLU	B	306	22.529	-40.067	-15.035	1.00	36.39
BBBBATOM	4893	CD	GLU	B	306	23.114	-41.388	-15.504	1.00	36.86
BBBBATOM	4894	OE1	GLU	B	306	22.468	-42.433	-15.289	1.00	36.59
BBBBATOM	4895	OE2	GLU	B	306	24.214	-41.378	-16.099	1.00	37.75
BBBBATOM	4896	C	GLU	B	306	21.531	-38.704	-11.552	1.00	35.50
BBBBATOM	4897	O	GLU	B	306	22.241	-37.984	-10.858	1.00	35.55
BBBBATOM	4898	N	GLN	B	307	20.612	-39.514	-11.048	1.00	38.41
BBBBATOM	4899	CA	GLN	B	307	20.377	-39.599	-9.613	1.00	40.54
BBBBATOM	4900	CB	GLN	B	307	19.397	-40.734	-9.322	1.00	40.99
BBBBATOM	4901	CG	GLN	B	307	18.896	-40.769	-7.896	1.00	42.76
BBBBATOM	4902	CD	GLN	B	307	17.879	-41.867	-7.681	1.00	44.33
BBBBATOM	4903	OE1	GLN	B	307	18.181	-43.051	-7.847	1.00	44.46
BBBBATOM	4904	NE2	GLN	B	307	16.659	-41.481	-7.318	1.00	45.30
BBBBATOM	4905	C	GLN	B	307	21.647	-39.784	-8.776	1.00	40.94
BBBBATOM	4906	O	GLN	B	307	21.796	-39.154	-7.732	1.00	41.24
BBBBATOM	4907	N	PRO	B	308	22.580	-40.648	-9.224	1.00	42.16
BBBBATOM	4908	CD	PRO	B	308	22.456	-41.593	-10.349	1.00	42.40
BBBBATOM	4909	CA	PRO	B	308	23.828	-40.891	-8.484	1.00	43.20
BBBBATOM	4910	CB	PRO	B	308	24.533	-41.954	-9.329	1.00	43.16

BBBBATOM	4911	CG	PRO	B	308	23.395	-42.708	-9.938	1.00	43.10
BBBBATOM	4912	C	PRO	B	308	24.719	-39.668	-8.250	1.00	43.82
BBBBATOM	4913	O	PRO	B	308	25.652	-39.724	-7.449	1.00	44.24
BBBBATOM	4914	N	GLN	B	309	24.442	-38.569	-8.944	1.00	44.04
BBBBATOM	4915	CA	GLN	B	309	25.247	-37.361	-8.787	1.00	43.46
BBBBATOM	4916	CB	GLN	B	309	26.071	-37.104	-10.056	1.00	44.98
BBBBATOM	4917	CG	GLN	B	309	27.183	-38.113	-10.329	1.00	46.93
BBBBATOM	4918	CD	GLN	B	309	26.683	-39.437	-10.885	1.00	47.93
BBBBATOM	4919	OE1	GLN	B	309	27.459	-40.376	-11.054	1.00	48.87
BBBBATOM	4920	NE2	GLN	B	309	25.388	-39.515	-11.179	1.00	49.17
BBBBATOM	4921	C	GLN	B	309	24.417	-36.119	-8.479	1.00	42.87
BBBBATOM	4922	O	GLN	B	309	24.955	-35.013	-8.404	1.00	43.33
BBBBATOM	4923	N	LEU	B	310	23.113	-36.297	-8.289	1.00	41.06
BBBBATOM	4924	CA	LEU	B	310	22.232	-35.166	-8.022	1.00	39.65
BBBBATOM	4925	CB	LEU	B	310	20.779	-35.549	-8.330	1.00	39.95
BBBBATOM	4926	CG	LEU	B	310	19.730	-34.437	-8.480	1.00	39.98
BBBBATOM	4927	CD1	LEU	B	310	19.545	-33.699	-7.166	1.00	41.39
BBBBATOM	4928	CD2	LEU	B	310	20.160	-33.472	-9.580	1.00	40.19
BBBBATOM	4929	C	LEU	B	310	22.342	-34.659	-6.591	1.00	38.83
BBBBATOM	4930	O	LEU	B	310	22.246	-35.428	-5.634	1.00	39.25
BBBBATOM	4931	N	SER	B	311	22.541	-33.354	-6.457	1.00	36.17
BBBBATOM	4932	CA	SER	B	311	22.660	-32.714	-5.154	1.00	34.90
BBBBATOM	4933	CB	SER	B	311	24.059	-32.928	-4.569	1.00	35.08
BBBBATOM	4934	OG	SER	B	311	25.022	-32.135	-5.248	1.00	33.92
BBBBATOM	4935	C	SER	B	311	22.434	-31.227	-5.357	1.00	33.51
BBBBATOM	4936	O	SER	B	311	22.476	-30.741	-6.485	1.00	33.60
BBBBATOM	4937	N	VAL	B	312	22.202	-30.509	-4.266	1.00	32.42
BBBBATOM	4938	CA	VAL	B	312	21.990	-29.074	-4.341	1.00	31.50
BBBBATOM	4939	CB	VAL	B	312	21.707	-28.482	-2.938	1.00	31.69
BBBBATOM	4940	CG1	VAL	B	312	21.546	-26.976	-3.023	1.00	31.54
BBBBATOM	4941	CG2	VAL	B	312	20.445	-29.106	-2.362	1.00	31.93
BBBBATOM	4942	C	VAL	B	312	23.228	-28.417	-4.946	1.00	31.40
BBBBATOM	4943	O	VAL	B	312	23.123	-27.612	-5.875	1.00	30.04
BBBBATOM	4944	N	ASP	B	313	24.406	-28.780	-4.444	1.00	30.18
BBBBATOM	4945	CA	ASP	B	313	25.642	-28.202	-4.957	1.00	29.61
BBBBATOM	4946	CB	ASP	B	313	26.840	-28.656	-4.120	1.00	32.36
BBBBATOM	4947	CG	ASP	B	313	26.817	-28.085	-2.718	1.00	34.21
BBBBATOM	4948	OD1	ASP	B	313	26.662	-26.855	-2.578	1.00	36.52
BBBBATOM	4949	OD2	ASP	B	313	26.958	-28.865	-1.751	1.00	38.92
BBBBATOM	4950	C	ASP	B	313	25.910	-28.516	-6.425	1.00	28.84
BBBBATOM	4951	O	ASP	B	313	26.442	-27.677	-7.146	1.00	28.96
BBBBATOM	4952	N	ALA	B	314	25.555	-29.719	-6.868	1.00	26.61
BBBBATOM	4953	CA	ALA	B	314	25.782	-30.099	-8.254	1.00	26.47
BBBBATOM	4954	CB	ALA	B	314	25.441	-31.575	-8.460	1.00	26.05
BBBBATOM	4955	C	ALA	B	314	24.928	-29.220	-9.174	1.00	25.78
BBBBATOM	4956	O	ALA	B	314	25.412	-28.714	-10.187	1.00	24.94
BBBBATOM	4957	N	VAL	B	315	23.661	-29.046	-8.815	1.00	25.00
BBBBATOM	4958	CA	VAL	B	315	22.755	-28.215	-9.612	1.00	25.33
BBBBATOM	4959	CB	VAL	B	315	21.305	-28.298	-9.088	1.00	24.74
BBBBATOM	4960	CG1	VAL	B	315	20.392	-27.382	-9.898	1.00	23.53
BBBBATOM	4961	CG2	VAL	B	315	20.810	-29.738	-9.172	1.00	25.69
BBBBATOM	4962	C	VAL	B	315	23.222	-26.764	-9.561	1.00	25.02
BBBBATOM	4963	O	VAL	B	315	23.398	-26.125	-10.590	1.00	25.73
BBBBATOM	4964	N	ALA	B	316	23.445	-26.251	-8.359	1.00	26.04
BBBBATOM	4965	CA	ALA	B	316	23.888	-24.872	-8.199	1.00	27.13
BBBBATOM	4966	CB	ALA	B	316	24.059	-24.545	-6.714	1.00	27.12
BBBBATOM	4967	C	ALA	B	316	25.185	-24.584	-8.955	1.00	28.17
BBBBATOM	4968	O	ALA	B	316	25.289	-23.572	-9.652	1.00	27.04
BBBBATOM	4969	N	ASN	B	317	26.178	-25.463	-8.823	1.00	28.72
BBBBATOM	4970	CA	ASN	B	317	27.444	-25.246	-9.518	1.00	28.52
BBBBATOM	4971	CB	ASN	B	317	28.493	-26.271	-9.081	1.00	31.30
BBBBATOM	4972	CG	ASN	B	317	28.940	-26.068	-7.645	1.00	34.01
BBBBATOM	4973	OD1	ASN	B	317	29.091	-24.933	-7.183	1.00	33.87
BBBBATOM	4974	ND2	ASN	B	317	29.170	-27.171	-6.933	1.00	35.63
BBBBATOM	4975	C	ASN	B	317	27.270	-25.310	-11.026	1.00	27.23
BBBBATOM	4976	O	ASN	B	317	27.887	-24.543	-11.765	1.00	26.36

BBBBATOM	4977	N	THR	B	318	26.424	-26.224	-11.482	1.00 26.95
BBBBATOM	4978	CA	THR	B	318	26.174	-26.371	-12.906	1.00 27.04
BBBBATOM	4979	CB	THR	B	318	25.203	-27.537	-13.189	1.00 27.91
BBBBATOM	4980	OG1	THR	B	318	25.843	-28.779	-12.872	1.00 30.24
BBBBATOM	4981	CG2	THR	B	318	24.784	-27.539	-14.655	1.00 27.49
BBBBATOM	4982	C	THR	B	318	25.579	-25.087	-13.480	1.00 26.50
BBBBATOM	4983	O	THR	B	318	26.085	-24.548	-14.465	1.00 26.71
BBBBATOM	4984	N	LEU	B	319	24.516	-24.588	-12.859	1.00 24.75
BBBBATOM	4985	CA	LEU	B	319	23.883	-23.370	-13.357	1.00 25.21
BBBBATOM	4986	CB	LEU	B	319	22.579	-23.090	-12.600	1.00 23.70
BBBBATOM	4987	CG	LEU	B	319	21.496	-24.153	-12.803	1.00 23.20
BBBBATOM	4988	CD1	LEU	B	319	20.384	-23.962	-11.785	1.00 22.93
BBBBATOM	4989	CD2	LEU	B	319	20.963	-24.065	-14.237	1.00 22.39
BBBBATOM	4990	C	LEU	B	319	24.814	-22.169	-13.253	1.00 25.23
BBBBATOM	4991	O	LEU	B	319	24.888	-21.368	-14.168	1.00 25.17
BBBBATOM	4992	N	ALA	B	320	25.540	-22.055	-12.147	1.00 24.41
BBBBATOM	4993	CA	ALA	B	320	26.445	-20.931	-11.957	1.00 24.59
BBBBATOM	4994	CB	ALA	B	320	27.069	-20.987	-10.547	1.00 24.46
BBBBATOM	4995	C	ALA	B	320	27.549	-20.865	-13.010	1.00 24.21
BBBBATOM	4996	O	ALA	B	320	28.091	-19.800	-13.281	1.00 24.35
BBBBATOM	4997	N	GLY	B	321	27.878	-22.005	-13.601	1.00 24.35
BBBBATOM	4998	CA.	GLY	B	321	28.934	-22.031	-14.591	1.00 24.34
BBBBATOM	4999	C	GLY	B	321	28.509	-21.642	-15.993	1.00 24.34
BBBBATOM	5000	O	GLY	B	321	29.345	-21.585	-16.890	1.00 24.63
BBBBATOM	5001	N	TRP	B	322	27.225	-21.357	-16.188	1.00 22.62
BBBBATOM	5002	CA	TRP	B	322	26.738	-21.007	-17.521	1.00 21.72
BBBBATOM	5003	CB	TRP	B	322	25.499	-21.841	-17.858	1.00 20.09
BBBBATOM	5004	CG	TRP	B	322	25.763	-23.318	-17.973	1.00 19.85
BBBBATOM	5005	CD2	TRP	B	322	24.789	-24.370	-17.939	1.00 19.16
BBBBATOM	5006	CE2	TRP	B	322	25.479	-25.584	-18.164	1.00 20.31
BBBBATOM	5007	CE3	TRP	B	322	23.403	-24.406	-17.742	1.00 19.35
BBBBATOM	5008	CD1	TRP	B	322	26.973	-23.925	-18.204	1.00 19.51
BBBBATOM	5009	NE1	TRP	B	322	26.806	-25.281	-18.323	1.00 18.84
BBBBATOM	5010	CZ2	TRP	B	322	24.825	-26.825	-18.198	1.00 20.00
BBBBATOM	5011	CZ3	TRP	B	322	22.749	-25.646	-17.775	1.00 19.90
BBBBATOM	5012	CH2	TRP	B	322	23.467	-26.836	-18.003	1.00 20.26
BBBBATOM	5013	C	TRP	B	322	26.422	-19.524	-17.722	1.00 21.61
BBBBATOM	5014	O	TRP	B	322	25.390	-19.030	-17.271	1.00 21.25
BBBBATOM	5015	N	SER	B	323	27.320	-18.824	-18.409	1.00 19.53
BBBBATOM	5016	CA	SER	B	323	27.141	-17.404	-18.692	1.00 19.04
BBBBATOM	5017	CB	SER	B	323	28.456	-16.807	-19.186	1.00 18.51
BBBBATOM	5018	OG	SER	B	323	28.793	-17.374	-20.447	1.00 16.33
BBBBATOM	5019	C	SER	B	323	26.099	-17.239	-19.799	1.00 18.26
BBBBATOM	5020	O	SER	B	323	25.690	-18.216	-20.426	1.00 16.71
BBBBATOM	5021	N	ARG	B	324	25.690	-15.999	-20.053	1.00 19.12
BBBBATOM	5022	CA	ARG	B	324	24.725	-15.741	-21.112	1.00 18.09
BBBBATOM	5023	CB	ARG	B	324	24.298	-14.268	-21.108	1.00 19.15
BBBBATOM	5024	CG	ARG	B	324	23.266	-13.973	-20.031	1.00 20.58
BBBBATOM	5025	CD	ARG	B	324	22.508	-12.662	-20.220	1.00 22.13
BBBBATOM	5026	NE	ARG	B	324	21.345	-12.641	-19.331	1.00 21.36
BBBBATOM	5027	CZ	ARG	B	324	20.268	-13.403	-19.510	1.00 21.63
BBBBATOM	5028	NH1	ARG	B	324	20.206	-14.224	-20.549	1.00 20.63
BBBBATOM	5029	NH2	ARG	B	324	19.269	-13.378	-18.633	1.00 22.19
BBBBATOM	5030	C	ARG	B	324	25.288	-16.145	-22.481	1.00 17.79
BBBBATOM	5031	O	ARG	B	324	24.540	-16.611	-23.341	1.00 17.56
BBBBATOM	5032	N	GLU	B	325	26.597	-15.975	-22.686	1.00 17.74
BBBBATOM	5033	CA	GLU	B	325	27.220	-16.368	-23.954	1.00 16.96
BBBBATOM	5034	CB	GLU	B	325	28.690	-15.907	-24.028	1.00 17.92
BBBBATOM	5035	CG	GLU	B	325	29.361	-16.398	-25.319	1.00 18.50
BBBBATOM	5036	CD	GLU	B	325	30.844	-16.068	-25.454	1.00 19.03
BBBBATOM	5037	OE1	GLU	B	325	31.446	-16.562	-26.433	1.00 18.89
BBBBATOM	5038	OE2	GLU	B	325	31.408	-15.325	-24.615	1.00 20.56
BBBBATOM	5039	C	GLU	B	325	27.164	-17.894	-24.110	1.00 16.65
BBBBATOM	5040	O	GLU	B	325	26.838	-18.428	-25.172	1.00 15.39
BBBBATOM	5041	N	THR	B	326	27.500	-18.603	-23.042	1.00 16.67
BBBBATOM	5042	CA	THR	B	326	27.460	-20.055	-23.070	1.00 16.39

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BBBBATOM	5043	CB	THR	B	326	27.967	−20.635	−21.725	1.00	16.62
BBBBATOM	5044	OG1	THR	B	326	29.346	−20.294	−21.561	1.00	18.31
BBBBATOM	5045	CG2	THR	B	326	27.804	−22.143	−21.690	1.00	18.20
BBBBATOM	5046	C	THR	B	326	26.034	−20.551	−23.321	1.00	17.40
BBBBATOM	5047	O	THR	B	326	25.817	−21.478	−24.107	1.00	16.65
BBBBATOM	5048	N	LEU	B	327	25.068	−19.932	−22.643	1.00	17.90
BBBBATOM	5049	CA	LEU	B	327	23.659	−20.305	−22.780	1.00	17.27
BBBBATOM	5050	CB	LEU	B	327	22.791	−19.514	−21.791	1.00	17.35
BBBBATOM	5051	CG	LEU	B	327	22.922	−19.919	−20.309	1.00	16.74
BBBBATOM	5052	CD1	LEU	B	327	22.192	−18.930	−19.416	1.00	14.82
BBBBATOM	5053	CD2	LEU	B	327	22.361	−21.312	−20.129	1.00	18.13
BBBBATOM	5054	C	LEU	B	327	23.145	−20.096	−24.198	1.00	17.58
BBBBATOM	5055	O	LEU	B	327	22.352	−20.899	−24.692	1.00	16.08
BBBBATOM	5056	N	LEU	B	328	23.584	−19.014	−24.845	1.00	17.87
BBBBATOM	5057	CA	LEU	B	328	23.175	−18.745	−26.222	1.00	17.39
BBBBATOM	5058	CB	LEU	B	328	23.706	−17.379	−26.690	1.00	17.84
BBBBATOM	5059	CG	LEU	B	328	23.475	−17.021	−28.173	1.00	18.65
BBBBATOM	5060	CD1	LEU	B	328	21.988	−17.112	−28.494	1.00	16.92
BBBBATOM	5061	CD2	LEU	B	328	23.984	−15.608	−28.460	1.00	18.47
BBBBATOM	5062	C	LEU	B	328	23.716	−19.868	−27.111	1.00	17.74
BBBBATOM	5063	O	LEU	B	328	23.003	−20.400	−27.953	1.00	17.59
BBBBATOM	5064	N	THR	B	329	24.977	−20.244	−26.910	1.00	20.12
BBBBATOM	5065	CA	THR	B	329	25.567	−21.335	−27.688	1.00	21.30
BBBBATOM	5066	CB	THR	B	329	27.069	−21.556	−27.336	1.00	22.69
BBBBATOM	5067	OG1	THR	B	329	27.866	−20.591	−28.029	1.00	25.80
BBBBATOM	5068	CG2	THR	B	329	27.533	−22.957	−27.757	1.00	24.48
BBBBATOM	5069	C	THR	B	329	24.819	−22.644	−27.457	1.00	20.40
BBBBATOM	5070	O	THR	B	329	24.552	−23.382	−28.398	1.00	20.34
BBBBATOM	5071	N	MET	B	330	24.494	−22.933	−26.200	1.00	20.31
BBBBATOM	5072	CA	MET	B	330	23.771	−24.153	−25.870	1.00	19.91
BBBBATOM	5073	CB	MET	B	330	23.642	−24.292	−24.350	1.00	20.88
BBBBATOM	5074	CG	MET	B	330	24.957	−24.571	−23.647	1.00	21.37
BBBBATOM	5075	SD	MET	B	330	24.805	−24.609	−21.855	1.00	22.76
BBBBATOM	5076	CE	MET	B	330	24.118	−26.250	−21.622	1.00	22.37
BBBBATOM	5077	C	MET	B	330	22.389	−24.149	−26.519	1.00	19.43
BBBBATOM	5078	O	MET	B	330	21.924	−25.167	−27.029	1.00	20.85
BBBBATOM	5079	N	ALA	B	331	21.737	−22.996	−26.504	1.00	18.81
BBBBATOM	5080	CA	ALA	B	331	20.412	−22.871	−27.098	1.00	18.49
BBBBATOM	5081	CB	ALA	B	331	19.868	−21.462	−26.859	1.00	17.16
BBBBATOM	5082	C	ALA	B	331	20.481	−23.162	−28.594	1.00	19.04
BBBBATOM	5083	O	ALA	B	331	19.644	−23.879	−29.130	1.00	18.16
BBBBATOM	5084	N	GLU	B	332	21.489	−22.613	−29.269	1.00	19.87
BBBBATOM	5085	CA	GLU	B	332	21.626	−22.827	−30.704	1.00	21.47
BBBBATOM	5086	CB	GLU	B	332	22.709	−21.912	−31.274	1.00	22.13
BBBBATOM	5087	CG	GLU	B	332	22.328	−20.455	−31.143	1.00	24.10
BBBBATOM	5088	CD	GLU	B	332	23.428	−19.522	−31.572	1.00	26.61
BBBBATOM	5089	OE1	GLU	B	332	24.594	−19.765	−31.197	1.00	26.92
BBBBATOM	5090	OE2	GLU	B	332	23.118	−18.542	−32.273	1.00	27.58
BBBBATOM	5091	C	GLU	B	332	21.921	−24.280	−31.025	1.00	22.44
BBBBATOM	5092	O	GLU	B	332	21.412	−24.814	−32.006	1.00	22.84
BBBBATOM	5093	N	ARG	B	333	22.739	−24.923	−30.200	1.00	22.30
BBBBATOM	5094	CA	ARG	B	333	23.040	−26.330	−30.408	1.00	23.77
BBBBATOM	5095	CB	ARG	B	333	24.117	−26.789	−29.427	1.00	25.03
BBBBATOM	5096	CG	ARG	B	333	25.503	−26.222	−29.737	1.00	26.79
BBBBATOM	5097	CD	ARG	B	333	26.443	−26.467	−28.570	1.00	28.88
BBBBATOM	5098	NE	ARG	B	333	27.810	−26.041	−28.846	1.00	29.09
BBBBATOM	5099	CZ	ARG	B	333	28.772	−26.001	−27.932	1.00	30.32
BBBBATOM	5100	NH1	ARG	B	333	28.514	−26.361	−26.678	1.00	32.07
BBBBATOM	5101	NH2	ARG	B	333	29.990	−25.596	−28.269	1.00	31.36
BBBBATOM	5102	C	ARG	B	333	21.763	−27.147	−30.218	1.00	23.13
BBBBATOM	5103	O	ARG	B	333	21.548	−28.151	−30.895	1.00	23.45
BBBBATOM	5104	N	ALA	B	334	20.907	−26.713	−29.299	1.00	22.82
BBBBATOM	5105	CA	ALA	B	334	19.648	−27.420	−29.063	1.00	22.88
BBBBATOM	5106	CB	ALA	B	334	18.915	−26.800	−27.882	1.00	22.08
BBBBATOM	5107	C	ALA	B	334	18.778	−27.333	−30.317	1.00	22.86
BBBBATOM	5108	O	ALA	B	334	18.285	−28.339	−30.827	1.00	21.38

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BBBBATOM	5109	N	ARG	B	335	18.602	-26.114	-30.815	1.00 23.14
BBBBATOM	5110	CA	ARG	B	335	17.795	-25.892	-32.002	1.00 23.54
BBBBATOM	5111	CB	ARG	B	335	17.815	-24.407	-32.361	1.00 25.17
BBBBATOM	5112	CG	ARG	B	335	16.804	-23.995	-33.418	1.00 26.90
BBBBATOM	5113	CD	ARG	B	335	15.381	-24.129	-32.891	1.00 30.87
BBBBATOM	5114	NE	ARG	B	335	14.435	-23.414	-33.736	1.00 33.71
BBBBATOM	5115	CZ	ARG	B	335	13.607	-22.469	-33.301	1.00 35.57
BBBBATOM	5116	NH1	ARG	B	335	13.601	-22.123	-32.016	1.00 34.54
BBBBATOM	5117	NH2	ARG	B	335	12.791	-21.862	-34.157	1.00 35.17
BBBBATOM	5118	C	ARG	B	335	18.348	-26.724	-33.163	1.00 23.86
BBBBATOM	5119	O	ARG	B	335	17.595	-27.360	-33.902	1.00 22.38
BBBBATOM	5120	N	ALA	B	336	19.671	-26.737	-33.297	1.00 25.17
BBBBATOM	5121	CA	ALA	B	336	20.330	-27.477	-34.372	1.00 26.85
BBBBATOM	5122	CB	ALA	B	336	21.830	-27.174	-34.374	1.00 26.27
BBBBATOM	5123	C	ALA	B	336	20.101	-28.985	-34.288	1.00 27.80
BBBBATOM	5124	O	ALA	B	336	20.052	-29.665	-35.308	1.00 27.33
BBBBATOM	5125	N	ALA	B	337	19.959	-29.501	-33.072	1.00 29.45
BBBBATOM	5126	CA	ALA	B	337	19.740	-30.925	-32.865	1.00 30.89
BBBBATOM	5127	CB	ALA	B	337	20.205	-31.320	-31.467	1.00 31.47
BBBBATOM	5128	C	ALA	B	337	18.267	-31.276	-33.047	1.00 32.47
BBBBATOM	5129	O	ALA	B	337	17.887	-32.445	-33.029	1.00 34.14
BBBBATOM	5130	N	SER	B	338	17.442	-30.254	-33.229	1.00 31.76
BBBBATOM	5131	CA	SER	B	338	16.008	-30.432	-33.408	1.00 32.41
BBBBATOM	5132	CB	SER	B	338	15.286	-29.140	-33.029	1.00 31.94
BBBBATOM	5133	OG	SER	B	338	13.921	-29.196	-33.385	1.00 34.53
BBBBATOM	5134	C	SER	B	338	15.593	-30.822	-34.829	1.00 33.16
BBBBATOM	5135	O	SER	B	338	16.274	-30.503	-35.801	1.00 32.25
BBBBATOM	5136	N	ILE	B	339	14.466	-31.523	-34.921	1.00 33.44
BBBBATOM	5137	CA	ILE	B	339	13.882	-31.941	-36.187	1.00 34.35
BBBBATOM	5138	CB	ILE	B	339	13.989	-33.472	-36.384	1.00 35.51
BBBBATOM	5139	CG2	ILE	B	339	13.271	-33.880	-37.658	1.00 35.53
BBBBATOM	5140	CG1	ILE	B	339	15.463	-33.887	-36.450	1.00 36.09
BBBBATOM	5141	CD1	ILE	B	339	15.688	-35.378	-36.667	1.00 37.71
BBBBATOM	5142	C	ILE	B	339	12.416	-31.518	-36.059	1.00 34.84
BBBBATOM	5143	O	ILE	B	339	11.601	-32.229	-35.479	1.00 35.09
BBBBATOM	5144	N	PRO	B	340	12.068	-30.344	-36.611	1.00 34.93
BBBBATOM	5145	CD	PRO	B	340	12.999	-29.525	-37.409	1.00 35.06
BBBBATOM	5146	CA	PRO	B	340	10.733	-29.730	-36.600	1.00 34.94
BBBBATOM	5147	CB	PRO	B	340	10.994	-28.349	-37.194	1.00 35.58
BBBBATOM	5148	CG	PRO	B	340	12.052	-28.642	-38.205	1.00 36.27
BBBBATOM	5149	C	PRO	B	340	9.551	-30.409	-37.284	1.00 34.07
BBBBATOM	5150	O	PRO	B	340	8.410	-30.222	-36.861	1.00 34.18
BBBBATOM	5151	N	ASP	B	341	9.803	-31.180	-38.334	1.00 33.42
BBBBATOM	5152	CA	ASP	B	341	8.711	-31.820	-39.056	1.00 33.33
BBBBATOM	5153	CB	ASP	B	341	8.802	-31.448	-40.536	1.00 35.03
BBBBATOM	5154	CG	ASP	B	341	10.101	-31.886	-41.159	1.00 37.02
BBBBATOM	5155	OD1	ASP	B	341	11.125	-31.907	-40.443	1.00 37.17
BBBBATOM	5156	OD2	ASP	B	341	10.102	-32.200	-42.367	1.00 40.57
BBBBATOM	5157	C	ASP	B	341	8.655	-33.336	-38.899	1.00 32.11
BBBBATOM	5158	O	ASP	B	341	8.377	-34.066	-39.854	1.00 30.74
BBBBATOM	5159	N	ALA	B	342	8.908	-33.807	-37.683	1.00 30.63
BBBBATOM	5160	CA	ALA	B	342	8.875	-35.238	-37.411	1.00 29.09
BBBBATOM	5161	CB	ALA	B	342	9.174	-35.496	-35.927	1.00 28.28
BBBBATOM	5162	C	ALA	B	342	7.530	-35.844	-37.792	1.00 28.32
BBBBATOM	5163	O	ALA	B	342	7.475	-36.901	-38.416	1.00 29.88
BBBBATOM	5164	N	THR	B	343	6.441	-35.177	-37.427	1.00 28.28
BBBBATOM	5165	CA	THR	B	343	5.115	-35.696	-37.744	1.00 28.55
BBBBATOM	5166	CB	THR	B	343	3.998	-34.765	-37.205	1.00 29.04
BBBBATOM	5167	OG1	THR	B	343	4.119	-34.642	-35.782	1.00 28.04
BBBBATOM	5168	CG2	THR	B	343	2.628	-35.330	-37.528	1.00 28.54
BBBBATOM	5169	C	THR	B	343	4.934	-35.882	-39.254	1.00 29.50
BBBBATOM	5170	O	THR	B	343	4.533	-36.952	-39.711	1.00 28.08
BBBBATOM	5171	N	GLU	B	344	5.234	-34.843	-40.030	1.00 30.76
BBBBATOM	5172	CA	GLU	B	344	5.085	-34.933	-41.480	1.00 32.00
BBBBATOM	5173	CB	GLU	B	344	5.414	-33.589	-42.142	1.00 34.02
BBBBATOM	5174	CG	GLU	B	344	4.412	-32.483	-41.814	1.00 38.27

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BBBBATOM	5175	CD	GLU	B	344	4.807	-31.661	-40.594	1.00	40.96
BBBBATOM	5176	OE1	GLU	B	344	5.252	-32.252	-39.582	1.00	41.33
BBBBATOM	5177	OE2	GLU	B	344	4.665	-30.419	-40.649	1.00	42.30
BBBBATOM	5178	C	GLU	B	344	5.970	-36.032	-42.056	1.00	31.14
BBBBATOM	5179	O	GLU	B	344	5.534	-36.805	-42.909	1.00	32.33
BBBBATOM	5180	N	ARG	B	345	7.209	-36.106	-41.587	1.00	30.66
BBBBATOM	5181	CA	ARG	B	345	8.138	-37.123	-42.067	1.00	31.44
BBBBATOM	5182	CB	ARG	B	345	9.494	-36.986	-41.376	1.00	33.54
BBBBATOM	5183	CG	ARG	B	345	10.293	-35.772	-41.793	1.00	37.73
BBBBATOM	5184	CD	ARG	B	345	11.716	-35.880	-41.284	1.00	40.70
BBBBATOM	5185	NE	ARG	B	345	12.580	-34.864	-41.873	1.00	44.36
BBBBATOM	5186	CZ	ARG	B	345	13.901	-34.841	-41.739	1.00	45.65
BBBBATOM	5187	NH1	ARG	B	345	14.514	-35.782	-41.031	1.00	46.05
BBBBATOM	5188	NH2	ARG	B	345	14.608	-33.881	-42.322	1.00	47.38
BBBBATOM	5189	C	ARG	B	345	7.626	-38.545	-41.854	1.00	30.89
BBBBATOM	5190	O	ARG	B	345	7.724	-39.387	-42.746	1.00	29.98
BBBBATOM	5191	N	VAL	B	346	7.086	-38.818	-40.670	1.00	29.72
BBBBATOM	5192	CA	VAL	B	346	6.578	-40.151	-40.384	1.00	28.61
BBBBATOM	5193	CB	VAL	B	346	6.197	-40.298	-38.885	1.00	27.90
BBBBATOM	5194	CG1	VAL	B	346	5.612	-41.680	-38.625	1.00	27.30
BBBBATOM	5195	CG2	VAL	B	346	7.419	-40.060	-38.024	1.00	27.32
BBBBATOM	5196	C	VAL	B	346	5.361	-40.435	-41.252	1.00	28.33
BBBBATOM	5197	O	VAL	B	346	5.248	-41.511	-41.847	1.00	28.30
BBBBATOM	5198	N	ALA	B	347	4.457	-39.465	-41.335	1.00	28.76
BBBBATOM	5199	CA	ALA	B	347	3.249	-39.617	-42.137	1.00	28.96
BBBBATOM	5200	CB	ALA	B	347	2.363	-38.387	-41.994	1.00	28.49
BBBBATOM	5201	C	ALA	B	347	3.596	-39.844	-43.606	1.00	30.26
BBBBATOM	5202	O	ALA	B	347	2.948	-40.641	-44.279	1.00	30.12
BBBBATOM	5203	N	ASN	B	348	4.613	-39.142	-44.098	1.00	32.77
BBBBATOM	5204	CA	ASN	B	348	5.035	-39.286	-45.493	1.00	34.56
BBBBATOM	5205	CB	ASN	B	348	6.045	-38.195	-45.868	1.00	35.68
BBBBATOM	5206	CG	ASN	B	348	5.384	-36.846	-46.123	1.00	37.21
BBBBATOM	5207	OD1	ASN	B	348	4.157	-36.719	-46.081	1.00	38.48
BBBBATOM	5208	ND2	ASN	B	348	6.199	-35.831	-46.393	1.00	38.38
BBBBATOM	5209	C	ASN	B	348	5.633	-40.668	-45.765	1.00	34.90
BBBBATOM	5210	O	ASN	B	348	5.433	-41.233	-46.841	1.00	34.59
BBBBATOM	5211	N	GLU	B	349	6.366	-41.212	-44.794	1.00	35.20
BBBBATOM	5212	CA	GLU	B	349	6.954	-42.540	-44.956	1.00	34.86
BBBBATOM	5213	CB	GLU	B	349	8.004	-42.814	-43.879	1.00	34.59
BBBBATOM	5214	CG	GLU	B	349	9.404	-42.385	-44.259	1.00	38.16
BBBBATOM	5215	CD	GLU	B	349	9.865	-42.992	-45.579	1.00	38.74
BBBBATOM	5216	OE1	GLU	B	349	9.806	-44.232	-45.753	1.00	40.12
BBBBATOM	5217	OE2	GLU	B	349	10.292	-42.225	-46.461	1.00	39.64
BBBBATOM	5218	C	GLU	B	349	5.872	-43.607	-44.895	1.00	33.96
BBBBATOM	5219	O	GLU	B	349	5.942	-44.621	-45.591	1.00	33.99
BBBBATOM	5220	N	VAL	B	350	4.875	-43.377	-44.051	1.00	33.91
BBBBATOM	5221	CA	VAL	B	350	3.767	-44.306	-43.919	1.00	33.79
BBBBATOM	5222	CB	VAL	B	350	2.848	-43.907	-42.744	1.00	33.70
BBBBATOM	5223	CG1	VAL	B	350	1.554	-44.695	-42.798	1.00	32.22
BBBBATOM	5224	CG2	VAL	B	350	3.568	-44.154	-41.425	1.00	32.24
BBBBATOM	5225	C	VAL	B	350	2.969	-44.274	-45.217	1.00	34.78
BBBBATOM	5226	O	VAL	B	350	2.411	-45.285	-45.645	1.00	34.85
BBBBATOM	5227	N	SER	B	351	2.925	-43.102	-45.844	1.00	35.34
BBBBATOM	5228	CA	SER	B	351	2.196	-42.946	-47.095	1.00	36.67
BBBBATOM	5229	CB	SER	B	351	2.024	-41.462	-47.425	1.00	37.32
BBBBATOM	5230	OG	SER	B	351	1.241	-41.292	-48.590	1.00	37.74
BBBBATOM	5231	C	SER	B	351	2.958	-43.639	-48.222	1.00	37.35
BBBBATOM	5232	O	SER	B	351	2.365	-44.309	-49.064	1.00	36.85
BBBBATOM	5233	N	ARG	B	352	4.277	-43.482	-48.223	1.00	37.89
BBBBATOM	5234	CA	ARG	B	352	5.114	-44.088	-49.251	1.00	40.03
BBBBATOM	5235	CB	ARG	B	352	6.557	-43.600	-49.114	1.00	41.58
BBBBATOM	5236	CG	ARG	B	352	7.470	-44.069	-50.232	1.00	44.46
BBBBATOM	5237	CD	ARG	B	352	8.906	-44.157	-49.759	1.00	47.36
BBBBATOM	5238	NE	ARG	B	352	9.097	-45.271	-48.832	1.00	49.57
BBBBATOM	5239	CZ	ARG	B	352	10.234	-45.524	-48.191	1.00	50.54
BBBBATOM	5240	NH1	ARG	B	352	11.287	-44.738	-48.372	1.00	50.88

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BBBBATOM   5241  NH2 ARG B 352      10.321 -46.566 -47.373  1.00 50.24
BBBBATOM   5242  C   ARG B 352       5.098 -45.613 -49.176  1.00 40.60
BBBBATOM   5243  O   ARG B 352       5.101 -46.292 -50.204  1.00 39.84
BBBBATOM   5244  N   VAL B 353       5.096 -46.143 -47.955  1.00 41.33
BBBBATOM   5245  CA  VAL B 353       5.089 -47.587 -47.737  1.00 42.78
BBBBATOM   5246  CB  VAL B 353       5.446 -47.927 -46.271  1.00 42.54
BBBBATOM   5247  CG1 VAL B 353       5.279 -49.420 -46.014  1.00 42.05
BBBBATOM   5248  CG2 VAL B 353       6.879 -47.509 -45.987  1.00 41.86
BBBBATOM   5249  C   VAL B 353       3.742 -48.206 -48.095  1.00 43.85
BBBBATOM   5250  O   VAL B 353       3.679 -49.343 -48.556  1.00 44.43
BBBBATOM   5251  N   ALA B 354       2.664 -47.465 -47.871  1.00 45.85
BBBBATOM   5252  CA  ALA B 354       1.336 -47.957 -48.212  1.00 47.24
BBBBATOM   5253  CB  ALA B 354       0.264 -47.043 -47.628  1.00 46.79
BBBBATOM   5254  C   ALA B 354       1.250 -47.971 -49.737  1.00 48.54
BBBBATOM   5255  O   ALA B 354       0.531 -48.780 -50.324  1.00 48.48
BBBBATOM   5256  N   ARG B 355       1.998 -47.068 -50.366  1.00 50.49
BBBBATOM   5257  CA  ARG B 355       2.035 -46.964 -51.824  1.00 52.71
BBBBATOM   5258  CB  ARG B 355       2.658 -45.633 -52.264  1.00 53.58
BBBBATOM   5259  CG  ARG B 355       1.998 -44.372 -51.730  1.00 55.08
BBBBATOM   5260  CD  ARG B 355       0.716 -44.014 -52.461  1.00 56.64
BBBBATOM   5261  NE  ARG B 355       0.112 -42.802 -51.907  1.00 57.43
BBBBATOM   5262  CZ  ARG B 355      -1.054 -42.296 -52.299  1.00 58.24
BBBBATOM   5263  NH1 ARG B 355      -1.758 -42.896 -53.252  1.00 58.53
BBBBATOM   5264  NH2 ARG B 355      -1.519 -41.186 -51.738  1.00 58.87
BBBBATOM   5265  C   ARG B 355       2.899 -48.099 -52.366  1.00 53.41
BBBBATOM   5266  O   ARG B 355       2.966 -48.319 -53.575  1.00 53.50
BBBBATOM   5267  N   ALA B 356       3.569 -48.805 -51.456  1.00 54.15
BBBBATOM   5268  CA  ALA B 356       4.453 -49.913 -51.809  1.00 54.93
BBBBATOM   5269  CB  ALA B 356       3.669 -51.004 -52.546  1.00 54.86
BBBBATOM   5270  C   ALA B 356       5.611 -49.417 -52.671  1.00 55.63
BBBBATOM   5271  O   ALA B 356       6.193 -50.178 -53.442  1.00 55.95
BBBBATOM   5272  N   LEU B 357       5.942 -48.136 -52.526  1.00 56.45
BBBBATOM   5273  CA  LEU B 357       7.023 -47.522 -53.289  1.00 57.81
BBBBATOM   5274  CB  LEU B 357       6.871 -45.997 -53.290  1.00 58.04
BBBBATOM   5275  CG  LEU B 357       5.595 -45.422 -53.915  1.00 58.29
BBBBATOM   5276  CD1 LEU B 357       5.624 -43.903 -53.820  1.00 58.36
BBBBATOM   5277  CD2 LEU B 357       5.485 -45.859 -55.370  1.00 58.62
BBBBATOM   5278  C   LEU B 357       8.391 -47.895 -52.729  1.00 58.46
BBBBATOM   5279  OT1 LEU B 357       9.244 -48.359 -53.514  1.00 58.97
BBBBATOM   5280  OT2 LEU B 357       8.601 -47.710 -51.512  1.00 58.97
BBBB
ATOM    5281  OH2 WAT W   1     -20.568  11.549  41.653  1.00 24.11
WATR
ATOM    5282  OH2 WAT W   4      -7.219 -67.275 -41.843  1.00 35.35
WATR
ATOM    5283  OH2 WAT W   5      20.119 -17.520 -22.473  1.00 21.13
WATR
ATOM    5284  OH2 WAT W   6      18.858 -19.701 -23.468  1.00 18.31
WATR
ATOM    5285  OH2 WAT W   7       2.329 -28.724 -15.978  1.00 27.32
WATR
ATOM    5286  OH2 WAT W   8       9.484 -48.435 -27.938  1.00 23.67
WATR
ATOM    5287  OH2 WAT W   9       7.645 -57.693 -27.177  1.00 21.03
WATR
ATOM    5288  OH2 WAT W  10      -1.542  -8.422   1.824  1.00 29.71
WATR
ATOM    5289  OH2 WAT W  11       5.875 -50.793 -32.396  1.00 20.21
WATR
ATOM    5290  OH2 WAT W  12      27.592 -18.174 -27.779  1.00 22.52
WATR
ATOM    5291  OH2 WAT W  13       7.842 -13.432 -21.178  1.00 25.85
WATR
ATOM    5292  OH2 WAT W  14       4.845 -57.924 -27.444  1.00 24.35
WATR
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ATOM   5293  OH2 WAT W  15     0.473 -58.751 -17.746  1.00 35.49
WATR
ATOM   5294  OH2 WAT W  16     7.998 -52.522 -25.785  1.00 22.34
WATR
ATOM   5295  OH2 WAT W  17    -8.656  11.300  18.872  1.00 23.81
WATR
ATOM   5296  OH2 WAT W  18     8.711 -45.913 -29.121  1.00 21.55
WATR
ATOM   5297  OH2 WAT W  19     2.957 -68.158 -38.242  1.00 29.43
WATR
ATOM   5298  OH2 WAT W  20    16.486 -11.742 -16.567  1.00 22.13
WATR
ATOM   5299  OH2 WAT W  21    -6.251  17.702  28.534  1.00 24.24
WATR
ATOM   5300  OH2 WAT W  22    12.670 -47.636 -24.808  1.00 25.87
WATR
ATOM   5301  OH2 WAT W  23     6.513 -15.597 -22.517  1.00 26.31
WATR
ATOM   5302  OH2 WAT W  24     7.536 -66.906 -21.753  1.00 21.48
WATR
ATOM   5303  OH2 WAT W  25   -29.060  13.621  26.406  1.00 21.08
WATR
ATOM   5304  OH2 WAT W  26    -5.240  10.154  13.527  1.00 29.62
WATR
ATOM   5305  OH2 WAT W  27    29.942 -20.139 -19.237  1.00 20.38
WATR
ATOM   5306  OH2 WAT W  28    18.996 -28.763 -24.427  1.00 20.28
WATR
ATOM   5307  OH2 WAT W  29     8.755 -51.080 -27.990  1.00 20.66
WATR
ATOM   5308  OH2 WAT W  30     4.215 -64.684 -43.328  1.00 39.67
WATR
ATOM   5309  OH2 WAT W  31    14.708 -11.936  -1.749  1.00 24.57
WATR
ATOM   5310  OH2 WAT W  32    28.140 -13.870 -21.266  1.00 18.93
WATR
ATOM   5311  OH2 WAT W  33     4.057  -1.221   9.809  1.00 32.30
WATR
ATOM   5312  OH2 WAT W  34     4.784 -56.759 -43.904  1.00 25.99
WATR
ATOM   5313  OH2 WAT W  35   -22.733  10.283  33.238  1.00 24.60
WATR
ATOM   5314  OH2 WAT W  36     0.540  14.225  10.932  1.00 26.89
WATR
ATOM   5315  OH2 WAT W  37    -7.560  11.931  12.593  1.00 27.76
WATR
ATOM   5316  OH2 WAT W  38    -7.966  17.043  30.555  1.00 20.04
WATR
ATOM   5317  OH2 WAT W  39     6.716 -55.314 -42.959  1.00 25.72
WATR
ATOM   5318  OH2 WAT W  40     6.833 -32.402  -3.845  1.00 32.49
WATR
ATOM   5319  OH2 WAT W  41    30.445 -20.104 -25.459  1.00 27.97
WATR
ATOM   5320  OH2 WAT W  42     1.475 -15.304 -22.128  1.00 30.57
WATR
ATOM   5321  OH2 WAT W  43    15.703 -42.835 -31.237  1.00 26.74
WATR
ATOM   5322  OH2 WAT W  44     7.131  -6.595 -18.003  1.00 29.47
WATR
ATOM   5323  OH2 WAT W  45    30.256 -23.202 -11.163  1.00 33.81
WATR
ATOM   5324  OH2 WAT W  46    -6.107 -66.004 -38.690  1.00 30.45
WATR
ATOM   5325  OH2 WAT W  47    17.631 -17.241  -5.864  1.00 28.69
WATR
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ATOM    5326   OH2 WAT W   48        13.436 -59.821 -27.855  1.00 28.71
WATR
ATOM    5327   OH2 WAT W   49        11.395 -15.293   2.925  1.00 29.36
WATR
ATOM    5328   OH2 WAT W   50        19.218 -21.377 -34.248  1.00 31.41
WATR
ATOM    5329   OH2 WAT W   51        11.973 -11.890 -15.788  1.00 35.59
WATR
ATOM    5330   OH2 WAT W   52         9.140  -8.260 -23.371  1.00 40.29
WATR
ATOM    5331   OH2 WAT W   53       -19.061  14.438  38.966  1.00 38.01
WATR
ATOM    5332   OH2 WAT W   54        -3.895 -70.510 -28.249  1.00 25.56
WATR
ATOM    5333   OH2 WAT W   55        20.909 -23.456 -34.213  1.00 26.74
WATR
ATOM    5334   OH2 WAT W   56        -8.505  11.136  10.323  1.00 30.97
WATR
ATOM    5335   OH2 WAT W   57        22.022 -15.529 -23.223  1.00 26.74
WATR
ATOM    5336   OH2 WAT W   58        13.860 -49.304 -42.490  1.00 27.91
WATR
ATOM    5337   OH2 WAT W   59        -9.455  -6.552  -9.720  1.00 41.70
WATR
ATOM    5338   OH2 WAT W   60        13.798 -49.732 -23.016  1.00 41.60
WATR
ATOM    5339   OH2 WAT W   61        15.881 -60.461 -31.910  1.00 48.66
WATR
ATOM    5340   OH2 WAT W   62        -9.797  12.718  13.997  1.00 29.14
WATR
ATOM    5341   OH2 WAT W   63        16.793   0.356  -6.115  1.00 26.17
WATR
ATOM    5342   OH2 WAT W   64         3.173  18.778  20.793  1.00 31.13
WATR
ATOM    5343   OH2 WAT W   65        13.433 -11.079   0.672  1.00 27.40
WATR
ATOM    5344   OH2 WAT W   66         3.118  -0.813   0.729  1.00 24.68
WATR
ATOM    5345   OH2 WAT W   67       -22.179   3.583  26.978  1.00 32.28
WATR
ATOM    5346   OH2 WAT W   68        24.433 -30.481  -1.783  1.00 41.91
WATR
ATOM    5347   OH2 WAT W   69         4.384 -66.131 -41.203  1.00 34.75
WATR
ATOM    5348   OH2 WAT W   70        20.398  -7.386  -4.280  1.00 30.85
WATR
ATOM    5349   OH2 WAT W   71        -2.444 -70.752 -22.067  1.00 25.46
WATR
ATOM    5350   OH2 WAT W   72        -3.963  -4.914  -5.711  1.00 29.67
WATR
ATOM    5351   OH2 WAT W   73        17.663 -11.040 -34.488  1.00 30.24
WATR
ATOM    5352   OH2 WAT W   74        21.404 -42.041 -26.621  1.00 31.41
WATRATOM    5353   OH2 WAT W   75        -1.110 -15.319  -1.089  1.00 31.51
WATRATOM    5354   OH2 WAT W   76         0.688  19.730  22.519  1.00 26.71
WATRATOM    5355   OH2 WAT W   77        12.113 -69.335 -26.593  1.00 27.11
WATRATOM    5356   OH2 WAT W   78        11.725 -25.065 -33.817  1.00 43.79
WATRATOM    5357   OH2 WAT W   79       -25.519   9.450  22.092  1.00 28.18
WATRATOM    5358   OH2 WAT W   80       -14.673   6.584  16.023  1.00 31.37
WATRATOM    5359   OH2 WAT W   81        -2.250  -0.253  -1.741  1.00 29.99
WATRATOM    5360   OH2 WAT W   82        -7.300  12.943   8.415  1.00 32.39
WATRATOM    5361   OH2 WAT W   83         1.712 -13.629 -13.904  1.00 34.08
WATRATOM    5362   OH2 WAT W   84         4.709 -17.478  -6.557  1.00 29.67
WATRATOM    5363   OH2 WAT W   85        10.070 -57.496 -44.450  1.00 48.39
WATRATOM    5364   OH2 WAT W   86         8.040 -30.281 -10.117  1.00 28.59
WATRATOM    5365   OH2 WAT W   87        -1.967 -32.372 -38.643  1.00 31.55
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WATRATOM   5366   OH2 WAT W   88    -3.178 -64.576 -25.506   1.00 33.66
WATRATOM   5367   OH2 WAT W   89    15.762  -9.860 -10.400   1.00 34.29
WATRATOM   5368   OH2 WAT W   90     5.654 -30.990 -27.758   1.00 35.84
WATRATOM   5369   OH2 WAT W   91    14.959 -46.096 -42.270   1.00 35.21
WATRATOM   5370   OH2 WAT W   92    10.137 -13.308  -9.753   1.00 32.65
WATRATOM   5371   OH2 WAT W   93    -4.480   6.624   6.614   1.00 27.37
WATRATOM   5372   OH2 WAT W   94   -14.574  22.522  18.870   1.00 49.48
WATRATOM   5373   OH2 WAT W   95   -11.031 -42.768 -39.637   1.00 37.63
WATRATOM   5374   OH2 WAT W   96     9.906 -35.479 -19.203   1.00 29.59
WATRATOM   5375   OH2 WAT W   97    -0.990  -0.781  36.951   1.00 37.27
WATRATOM   5376   OH2 WAT W   98   -11.422   9.059  11.252   1.00 30.43
WATRATOM   5377   OH2 WAT W   99     8.118 -36.710 -22.371   1.00 34.85
WATRATOM   5378   OH2 WAT W  100    12.414 -67.326 -22.791   1.00 31.24
WATRATOM   5379   OH2 WAT W  101    28.541 -24.603 -31.049   1.00 40.14
WATRATOM   5380   OH2 WAT W  102    16.276 -10.934  -3.673   1.00 33.80
WATRATOM   5381   OH2 WAT W  103    30.979 -13.264 -22.953   1.00 24.73
WATRATOM   5382   OH2 WAT W  104    12.759 -31.636 -31.838   1.00 26.40
WATRATOM   5383   OH2 WAT W  105    23.507 -29.661 -32.187   1.00 29.62
WATRATOM   5384   OH2 WAT W  106    21.292 -13.141 -24.874   1.00 37.83
WATRATOM   5385   OH2 WAT W  107    10.171 -32.960 -15.580   1.00 26.59
WATRATOM   5386   OH2 WAT W  108    -2.207   2.376   2.034   1.00 27.55
WATRATOM   5387   OH2 WAT W  109    -6.984  22.588  16.082   1.00 39.01
WATRATOM   5388   OH2 WAT W  110    14.308 -11.038 -15.406   1.00 26.48
WATRATOM   5389   OH2 WAT W  111    10.612   9.749  24.161   1.00 40.18
WATRATOM   5390   OH2 WAT W  112     2.406 -15.823 -10.196   1.00 27.61
WATRATOM   5391   OH2 WAT W  113     6.310 -68.984 -20.661   1.00 40.25
WATRATOM   5392   OH2 WAT W  114    14.379 -10.930  -8.565   1.00 35.86
WATRATOM   5393   OH2 WAT W  115    24.183 -35.475 -30.338   1.00 35.17
WATRATOM   5394   OH2 WAT W  116    21.897 -31.717  -1.243   1.00 47.61
WATRATOM   5395   OH2 WAT W  117    24.065 -17.545 -13.707   1.00 32.24
WATRATOM   5396   OH2 WAT W  118    16.772 -51.926 -25.940   1.00 38.66
WATRATOM   5397   OH2 WAT W  119    -5.862   6.629   4.446   1.00 39.57
WATRATOM   5398   OH2 WAT W  120    14.133 -57.303 -28.159   1.00 30.19
WATRATOM   5399   OH2 WAT W  121   -16.538  -6.724  21.638   1.00 40.50
WATRATOM   5400   OH2 WAT W  122    19.669 -18.487 -33.216   1.00 38.38
WATRATOM   5401   OH2 WAT W  123    15.481   1.078  -4.048   1.00 32.28
WATRATOM   5402   OH2 WAT W  124    20.395 -13.033  -2.072   1.00 49.69
WATRATOM   5403   OH2 WAT W  125    15.526  -1.437 -15.842   1.00 36.06
WATRATOM   5404   OH2 WAT W  126     7.297 -29.419  -1.509   1.00 34.75
WATRATOM   5405   OH2 WAT W  127     9.994 -12.069 -21.013   1.00 32.21
WATRATOM   5406   OH2 WAT W  128    17.433 -42.825 -16.713   1.00 31.02
WATRATOM   5407   OH2 WAT W  129   -15.855  20.882  21.019   1.00 44.11
WATRATOM   5408   OH2 WAT W  130    -6.351  -7.687 -14.067   1.00 35.04
WATRATOM   5409   OH2 WAT W  131     7.954 -17.872  -1.475   1.00 28.45
WATRATOM   5410   OH2 WAT W  132    13.526 -34.593 -31.844   1.00 31.12
WATRATOM   5411   OH2 WAT W  133     9.992 -41.228 -23.098   1.00 26.45
WATRATOM   5412   OH2 WAT W  134     8.434  18.132  16.019   1.00 32.97
WATRATOM   5413   OH2 WAT W  135    -1.208 -33.658 -36.216   1.00 38.33
WATRATOM   5414   OH2 WAT W  136   -14.502   9.100  12.433   1.00 43.21
WATRATOM   5415   OH2 WAT W  137    14.394 -43.675 -17.325   1.00 32.32
WATRATOM   5416   OH2 WAT W  138    -4.809 -30.333 -46.416   1.00 42.65
WATRATOM   5417   OH2 WAT W  139    18.861 -35.072 -35.671   1.00 43.56
WATRATOM   5418   OH2 WAT W  140   -10.162 -60.139 -32.862   1.00 35.41
WATRATOM   5419   OH2 WAT W  141     6.740 -32.411 -35.303   1.00 38.57
WATRATOM   5420   OH2 WAT W  142   -12.257 -60.854 -39.307   1.00 32.90
WATRATOM   5421   OH2 WAT W  143    18.910 -40.984 -13.084   1.00 43.43
WATRATOM   5422   OH2 WAT W  144    18.857 -49.375 -28.645   1.00 31.34
WATRATOM   5423   OH2 WAT W  145     0.235 -17.424 -16.608   1.00 38.85
WATRATOM   5424   OH2 WAT W  146    14.236 -11.252 -24.086   1.00 27.79
WATRATOM   5425   OH2 WAT W  147    31.513 -22.336 -22.128   1.00 43.18
WATRATOM   5426   OH2 WAT W  148    -5.314 -70.396 -26.090   1.00 43.91
WATRATOM   5427   OH2 WAT W  149    -7.717 -64.969 -36.808   1.00 26.30
WATRATOM   5428   OH2 WAT W  150    22.584 -12.594  -4.179   1.00 46.91
WATRATOM   5429   OH2 WAT W  151   -12.388   9.493  36.619   1.00 32.82
WATRATOM   5430   OH2 WAT W  152   -14.517  16.479  37.760   1.00 39.52
WATRATOM   5431   OH2 WAT W  153   -10.095 -34.647 -29.068   1.00 41.08
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WATRATOM	5432	OH2	WAT	W	154	-5.233	-4.134	31.160	1.00 35.31
WATRATOM	5433	OH2	WAT	W	155	-6.322	11.278	-1.883	1.00 35.75
WATRATOM	5434	OH2	WAT	W	156	10.262	-9.572	-16.736	1.00 42.40
WATRATOM	5435	OH2	WAT	W	157	22.929	-10.414	-23.566	1.00 36.66
WATRATOM	5436	OH2	WAT	W	158	-15.987	3.994	16.559	1.00 37.22
WATRATOM	5437	OH2	WAT	W	159	13.385	-44.923	-46.826	1.00 41.55
WATRATOM	5438	OH2	WAT	W	160	26.508	-13.616	-18.049	1.00 25.93
WATRATOM	5439	OH2	WAT	W	161	4.671	-66.907	-17.861	1.00 31.54
WATRATOM	5440	OH2	WAT	W	162	-12.589	12.262	11.825	1.00 32.71
WATRATOM	5441	OH2	WAT	W	163	13.899	-62.269	-25.144	1.00 30.71
WATRATOM	5442	OH2	WAT	W	164	-31.053	15.663	19.272	1.00 30.19
WATRATOM	5443	OH2	WAT	W	165	9.797	-47.899	-25.140	1.00 26.79
WATRATOM	5444	OH2	WAT	W	166	0.877	-51.774	-25.619	1.00 30.02
WATRATOM	5445	OH2	WAT	W	167	-17.088	16.246	37.180	1.00 25.63
WATRATOM	5446	OH2	WAT	W	168	0.855	-52.086	-22.078	1.00 40.99
WATRATOM	5447	OH2	WAT	W	169	-14.873	18.295	21.203	1.00 40.28
WATRATOM	5448	OH2	WAT	W	170	11.913	-62.134	-35.641	1.00 41.33
WATRATOM	5449	OH2	WAT	W	171	25.783	-23.984	-33.162	1.00 44.03
WATRATOM	5450	OH2	WAT	W	172	7.169	-50.047	-23.737	1.00 47.85
WATRATOM	5451	OH2	WAT	W	173	20.074	-42.845	-14.939	1.00 32.87
WATRATOM	5452	OH2	WAT	W	174	8.765	5.909	9.193	1.00 34.30
WATRATOM	5453	OH2	WAT	W	175	-4.953	-64.494	-45.351	1.00 47.11
WATRATOM	5454	OH2	WAT	W	176	11.889	-61.263	-22.531	1.00 36.63
WATRATOM	5455	OH2	WAT	W	177	2.149	-49.169	-24.836	1.00 39.21
WATRATOM	5456	OH2	WAT	W	178	-14.051	6.399	13.353	1.00 39.89
WATRATOM	5457	OH2	WAT	W	179	8.488	-46.760	-23.118	1.00 45.24
WATRATOM	5458	OH2	WAT	W	180	-1.152	-23.348	-11.975	1.00 30.36
WATRATOM	5459	OH2	WAT	W	181	-7.002	3.531	7.051	1.00 44.50
WATRATOM	5460	OH2	WAT	W	182	-12.320	-54.772	-29.990	1.00 38.61
WATRATOM	5461	OH2	WAT	W	183	6.790	-54.559	-47.733	1.00 44.05
WATRATOM	5462	OH2	WAT	W	184	26.305	-38.240	-19.177	1.00 39.53
WATRATOM	5463	OH2	WAT	W	185	20.402	-58.179	-34.391	1.00 46.11
WATRATOM	5464	OH2	WAT	W	186	8.061	-31.341	-19.653	1.00 41.37
WATRATOM	5465	OH2	WAT	W	187	-7.549	-15.619	-5.482	1.00 40.60
WATRATOM	5466	OH2	WAT	W	188	-31.099	11.941	25.471	1.00 38.80
WATRATOM	5467	OH2	WAT	W	189	28.566	-25.441	-15.103	1.00 34.75
WATRATOM	5468	OH2	WAT	W	190	-5.613	-40.109	-50.158	1.00 49.21
WATRATOM	5469	OH2	WAT	W	191	17.024	-13.428	1.709	1.00 39.93
WATRATOM	5470	OH2	WAT	W	192	-22.114	10.176	37.673	1.00 32.53
WATRATOM	5471	OH2	WAT	W	193	10.204	-29.330	-20.066	1.00 27.24
WATRATOM	5472	OH2	WAT	W	194	27.893	-25.793	-21.862	1.00 38.97
WATRATOM	5473	OH2	WAT	W	195	-5.582	17.681	32.898	1.00 43.64
WATRATOM	5474	OH2	WAT	W	196	23.004	-45.224	-27.870	1.00 43.04
WATRATOM	5475	OH2	WAT	W	197	5.189	-58.857	-25.016	1.00 28.15
WATRATOM	5476	OH2	WAT	W	198	-7.740	-56.165	-24.052	1.00 35.98
WATRATOM	5477	OH2	WAT	W	199	-8.156	24.723	26.733	1.00 45.54
WATRATOM	5478	OH2	WAT	W	200	23.286	-32.333	-33.400	1.00 38.12
WATRATOM	5479	OH2	WAT	W	201	30.646	-14.180	-20.528	1.00 31.01
WATRATOM	5480	OH2	WAT	W	202	-8.238	-4.609	29.299	1.00 39.76
WATRATOM	5481	OH2	WAT	W	203	19.370	0.814	-7.532	1.00 35.83
WATRATOM	5482	OH2	WAT	W	204	0.885	-27.619	-1.442	1.00 47.04
WATRATOM	5483	OH2	WAT	W	205	16.084	-56.649	-26.382	1.00 45.97
WATRATOM	5484	OH2	WAT	W	206	-0.698	-19.360	-9.869	1.00 37.53
WATRATOM	5485	OH2	WAT	W	207	0.682	-14.985	-15.794	1.00 33.35
WATRATOM	5486	OH2	WAT	W	208	1.646	17.427	31.991	1.00 40.39
WATRATOM	5487	OH2	WAT	W	209	-21.611	1.533	20.359	1.00 31.04
WATRATOM	5488	OH2	WAT	W	210	-5.143	-55.137	-45.825	1.00 30.17
WATRATOM	5489	OH2	WAT	W	211	-9.645	13.045	37.660	1.00 42.93
WATRATOM	5490	OH2	WAT	W	212	22.096	-11.242	-30.224	1.00 48.12
WATRATOM	5491	OH2	WAT	W	213	-5.759	2.610	-15.984	1.00 41.67
WATRATOM	5492	OH2	WAT	W	214	-4.323	7.731	-7.331	1.00 37.92
WATRATOM	5493	OH2	WAT	W	215	-5.450	7.197	10.632	1.00 33.99
WATRATOM	5494	OH2	WAT	W	216	2.330	-32.635	-34.500	1.00 38.85
WATRATOM	5495	OH2	WAT	W	217	-26.827	16.219	13.451	1.00 38.12
WATRATOM	5496	OH2	WAT	W	218	10.887	-51.427	-23.191	1.00 39.81
WATRATOM	5497	OH2	WAT	W	219	-9.020	19.746	-3.698	1.00 46.58

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WATRATOM   5498   OH2 WAT W 220      9.054     6.622    -0.709   1.00 34.14
WATRATOM   5499   OH2 WAT W 221      4.173    -7.985   -23.786   1.00 32.75
WATRATOM   5500   OH2 WAT W 222      0.983    16.806     3.910   1.00 40.83
WATRATOM   5501   OH2 WAT W 223      2.222   -16.848    -6.783   1.00 33.50
WATRATOM   5502   OH2 WAT W 224     13.627     1.072   -15.114   1.00 37.51
WATRATOM   5503   OH2 WAT W 225     12.533   -14.212    -9.007   1.00 38.40
WATRATOM   5504   OH2 WAT W 226      1.404    -7.852     5.396   1.00 38.55
WATRATOM   5505   OH2 WAT W 227     31.159   -24.354   -31.143   1.00 37.67
WATRATOM   5506   OH2 WAT W 228    -13.047   -60.728   -42.282   1.00 42.18
WATRATOM   5507   OH2 WAT W 229      8.956   -37.681   -16.765   1.00 41.45
WATRATOM   5508   OH2 WAT W 230     28.749   -13.637   -16.860   1.00 42.34
WATRATOM   5509   OH2 WAT W 231     -4.461    19.451     8.684   1.00 36.17
WATRATOM   5510   OH2 WAT W 232     -9.785   -66.504   -35.701   1.00 44.07
WATRATOM   5511   OH2 WAT W 233     10.673   -41.619   -20.678   1.00 36.58
WATRATOM   5512   OH2 WAT W 234    -15.694     1.684    32.613   1.00 44.04
WATRATOM   5513   OH2 WAT W 235      3.345     1.229     9.738   1.00 35.70
WATRATOM   5514   OH2 WAT W 236     -6.256   -68.913   -30.401   1.00 36.72
WATRATOM   5515   OH2 WAT W 237     28.344   -21.326   -30.399   1.00 36.45
WATRATOM   5516   OH2 WAT W 238      2.876   -34.368   -17.344   1.00 42.48
WATRATOM   5517   OH2 WAT W 239     15.355   -11.202     2.371   1.00 38.84
WATRATOM   5518   OH2 WAT W 240     27.066   -22.336    -6.437   1.00 37.37
WATRATOM   5519   OH2 WAT W 241      2.222    18.464    26.994   1.00 35.75
WATRATOM   5520   OH2 WAT W 242     15.052    -9.829   -31.019   1.00 44.31
WATRATOM   5521   OH2 WAT W 243     10.351   -67.649   -21.184   1.00 35.79
WATRATOM   5522   OH2 WAT W 244    -13.173    14.269    38.605   1.00 41.50
WATRATOM   5523   OH2 WAT W 245     -7.569     9.658     0.793   1.00 37.62
WATRATOM   5524   OH2 WAT W 246     -2.167   -47.395   -19.605   1.00 45.90
WATRATOM   5525   OH2 WAT W 247      7.166     2.400    15.830   1.00 42.90
WATRATOM   5526   OH2 WAT W 248    -11.231   -10.901   -10.057   1.00 45.28
WATRATOM   5527   OH2 WAT W 249      5.684   -16.094   -26.796   1.00 44.76
WATRATOM   5528   OH2 WAT W 250     -4.745     3.667   -18.932   1.00 46.20
WATRATOM   5529   OH2 WAT W 251     -0.505   -22.136    -9.079   1.00 42.89
WATRATOM   5530   OH2 WAT W 252     16.668   -37.987    -7.767   1.00 35.76
WATRATOM   5531   OH2 WAT W 253      2.454   -18.256   -26.130   1.00 43.33
WATRATOM   5532   OH2 WAT W 254     -8.367   -39.960   -21.638   1.00 43.07
WATRATOM   5533   OH2 WAT W 255     15.642     7.805     9.633   1.00 47.78
WATRATOM   5534   OH2 WAT W 256     13.660   -24.331     1.932   1.00 42.50
WATRATOM   5535   OH2 WAT W 257     11.567    -6.104   -23.359   1.00 37.10
WATRATOM   5536   OH2 WAT W 258     18.941   -16.698     0.528   1.00 40.97
WATRATOM   5537   OH2 WAT W 259    -11.441   -63.514   -39.126   1.00 43.17
WATRATOM   5538   OH2 WAT W 260     28.664   -39.605   -22.853   1.00 42.65
WATRATOM   5539   OH2 WAT W 261      6.795    -6.961    31.114   1.00 38.28
WATRATOM   5540   OH2 WAT W 262      7.077   -14.349   -24.858   1.00 41.00
WATRATOM   5541   OH2 WAT W 263     -2.259   -48.991   -29.099   1.00 34.96
WATRATOM   5542   OH2 WAT W 264     21.812   -44.128   -35.641   1.00 44.51
WATRATOM   5543   OH2 WAT W 265    -27.570     4.389    13.296   1.00 48.63
WATRATOM   5544   OH2 WAT W 266     13.573   -27.185     0.220   1.00 43.56
WATRATOM   5545   OH2 WAT W 267     16.549     8.451   -13.582   1.00 44.84
WATRATOM   5546   OH2 WAT W 268     -9.142     9.107    36.872   1.00 37.66
WATRATOM   5547   OH2 WAT W 269      5.648   -11.797   -24.893   1.00 45.79
WATRATOM   5548   OH2 WAT W 270      3.619   -14.850   -23.652   1.00 34.09
WATRATOM   5549   OH2 WAT W 271     -8.129   -11.098   -16.064   1.00 39.37
WATRATOM   5550   OH2 WAT W 272    -17.342     8.563     9.979   1.00 46.38
WATRATOM   5551   OH2 WAT W 273      8.798   -36.348   -46.119   1.00 37.71
WATRATOM   5552   OH2 WAT W 274      9.190   -10.509   -35.865   1.00 45.80
WATRATOM   5553   OH2 WAT W 275     13.545   -13.441     3.898   1.00 42.83
WATRATOM   5554   OH2 WAT W 276     -7.844     0.944    -2.560   1.00 46.27
WATRATOM   5555   OH2 WAT W 277      0.478   -47.721   -55.170   1.00 46.25
WATRATOM   5556   OH2 WAT W 278     24.658   -18.359   -11.005   1.00 36.33
WATRATOM   5557   OH2 WAT W 279     -4.675    21.561    12.155   1.00 37.17
WATRATOM   5558   OH2 WAT W 280      0.382    20.486     4.930   1.00 41.40
WATRATOM   5559   OH2 WAT W 281      5.919    18.010    25.033   1.00 41.72
WATRATOM   5560   OH2 WAT W 282     -2.987   -63.751   -22.983   1.00 43.76
WATRATOM   5561   OH2 WAT W 283      8.990   -33.134   -17.898   1.00 40.17
WATRATOM   5562   OH2 WAT W 284      0.155   -61.872   -48.384   1.00 49.87
WATRATOM   5563   OH2 WAT W 285    -10.443   -56.965   -24.681   1.00 48.02
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WATRATOM    5564    OH2 WAT W 286        18.915 -33.048  -3.930  1.00 37.81
WATRATOM    5565    OH2 WAT W 287       -16.181  11.706  12.277  1.00 41.77
WATRATOM    5566    OH2 WAT W 288         7.197   7.180  10.953  1.00 46.19
WATRATOM    5567    OH2 WAT W 289        31.934 -26.155 -26.053  1.00 38.77
WATRATOM    5568    OH2 WAT W 290       -15.232  -0.248  11.315  1.00 40.14
WATRATOM    5569    OH2 WAT W 291         9.450 -27.963  -1.396  1.00 41.29
WATRATOM    5570    OH2 WAT W 292        -1.800  13.139  -9.983  1.00 41.60
WATRATOM    5571    OH2 WAT W 293        -7.766   5.988   9.798  1.00 40.11
WATRATOM    5572    OH2 WAT W 294         7.973   4.338  14.321  1.00 39.97
WATRATOM    5573    OH2 WAT W 295        23.449 -40.563 -27.347  1.00 40.59
WATRATOM    5574    OH2 WAT W 296        -3.537 -28.260 -15.925  1.00 42.10
WATRATOM    5575    OH2 WAT W 297        28.052 -32.620 -12.168  1.00 48.03
WATRATOM    5576    OH2 WAT W 298        20.655 -43.315 -28.829  1.00 40.17
WATR
ATOM    5577   S   SO4 S    1     1.273 -70.953 -23.009  1.00 22.99
SO4
ATOM    5578   O1  SO4 S    1     1.720 -71.882 -24.053  1.00 21.18
SO4
ATOM    5579   O2  SO4 S    1     0.908 -69.659 -23.626  1.00 22.47
SO4
ATOM    5580   O3  SO4 S    1     2.337 -70.752 -22.018  1.00 23.88
SO4
ATOM    5581   O4  SO4 S    1     0.088 -71.522 -22.328  1.00 22.50
SO4
TEREND
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TABLE 2 ATOMIC COORDINATES OF E.COLI MURG C-ALPHA

BACKBONE ATOMS

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ATOM   2649   CA   LYS B    7    -6.512 -45.403 -47.519  1.00 45.28  BBBB
ATOM   2651   CA   ARG B    8    -6.682 -47.303 -44.240  1.00 38.63  BBBB
ATOM   2662   CA   LEU B    9    -4.094 -47.039 -41.477  1.00 30.88  BBBB
ATOM   2670   CA   MET B   10    -4.048 -49.055 -38.275  1.00 26.66  BBBB
ATOM   2678   CA   VAL B   11    -1.982 -47.605 -35.449  1.00 23.16  BBBB
ATOM   2685   CA   MET B   12    -0.523 -49.707 -32.613  1.00 24.54  BBBB
ATOM   2693   CA   ALA B   13     0.508 -47.410 -29.752  1.00 29.43  BBBB
ATOM   2698   CA   GLY B   14    -0.513 -47.804 -26.120  1.00 33.82  BBBB
ATOM   2702   CA   GLY B   15    -0.700 -45.047 -23.536  1.00 36.08  BBBB
ATOM   2706   CA   THR B   16     1.920 -46.787 -21.421  1.00 38.51  BBBB
ATOM   2713   CA   GLY B   17     5.367 -45.567 -22.392  1.00 36.57  BBBB
ATOM   2717   CA   GLY B   18     3.631 -42.529 -23.872  1.00 33.48  BBBB
ATOM   2721   CA   HIS B   19     3.548 -43.865 -27.435  1.00 28.22  BBBB
ATOM   2731   CA   VAL B   20    -0.098 -42.894 -27.965  1.00 27.77  BBBB
ATOM   2738   CA   PHE B   21     0.517 -39.136 -28.160  1.00 29.00  BBBB
ATOM   2750   CA   PRO B   22     2.986 -39.252 -31.086  1.00 26.12  BBBB
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ATOM   2853   CA   GLN B   36    -9.175 -43.535 -42.402  1.00 35.40  BBBB
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ATOM   2894   CA   LEU B   40    -5.200 -51.364 -32.026  1.00 24.71  BBBB
ATOM   2902   CA   GLY B   41    -4.691 -51.450 -28.257  1.00 23.47  BBBB
ATOM   2906   CA   THR B   42    -5.787 -53.141 -25.027  1.00 29.84  BBBB
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ATOM   3056   CA   ILE B   61    -6.832 -57.616 -28.269  1.00 28.55  BBBB
ATOM   3064   CA   ARG B   62    -5.709 -59.416 -25.133  1.00 30.76  BBBB
ATOM   3075   CA   ILE B   63    -2.036 -59.770 -24.231  1.00 31.38  BBBB
ATOM   3083   CA   SER B   64    -2.356 -60.520 -20.505  1.00 37.51  BBBB
ATOM   3089   CA   GLY B   65     0.679 -62.355 -19.199  1.00 37.13  BBBB
ATOM   3093   CA   LEU B   66     2.591 -61.413 -22.355  1.00 33.17  BBBB
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ATOM   3116   CA   LYS B  69     8.238 -60.463 -22.796  1.00 23.93  BBBB
ATOM   3125   CA   GLY B  70    10.755 -60.229 -25.636  1.00 22.26  BBBB
ATOM   3129   CA   ILE B  71    10.357 -62.386 -28.762  1.00 23.55  BBBB
ATOM   3137   CA   LYS B  72    12.038 -65.491 -27.343  1.00 24.92  BBBB
ATOM   3146   CA   ALA B  73     9.839 -65.306 -24.233  1.00 21.18  BBBB
ATOM   3151   CA   LEU B  74     6.745 -64.762 -26.387  1.00 19.36  BBBB
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ATOM   3167   CA   ALA B  76     7.996 -69.726 -25.374  1.00 21.72  BBBB
ATOM   3172   CA   ALA B  77     4.289 -69.121 -24.655  1.00 21.07  BBBB
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ATOM   3184   CA   LEU B  79    -0.896 -70.728 -26.783  1.00 21.32  BBBB
ATOM   3192   CA   ARG B  80    -0.980 -67.115 -25.637  1.00 21.30  BBBB
ATOM   3203   CA   ILE B  81     1.113 -65.621 -28.421  1.00 19.47  BBBB
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ATOM   3222   CA   ASN B  83    -4.150 -66.332 -29.577  1.00 20.90  BBBB
ATOM   3230   CA   ALA B  84    -3.177 -62.647 -29.484  1.00 19.30  BBBB
ATOM   3235   CA   TRP B  85    -1.820 -63.111 -33.032  1.00 20.56  BBBB
ATOM   3249   CA   ARG B  86    -5.140 -64.660 -34.166  1.00 23.28  BBBB
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ATOM   3298   CA   MET B  92    -6.872 -56.693 -39.717  1.00 29.03  BBBB
ATOM   3306   CA   LYS B  93    -8.735 -59.038 -42.050  1.00 33.20  BBBB
ATOM   3315   CA   ALA B  94   -11.943 -57.157 -41.183  1.00 33.62  BBBB
ATOM   3320   CA   TYR B  95   -10.504 -53.620 -41.224  1.00 33.83  BBBB
ATOM   3332   CA   LYS B  96    -8.104 -54.327 -44.122  1.00 33.85  BBBB
ATOM   3342   CA   PRO B  97    -5.490 -51.623 -43.419  1.00 31.82  BBBB
ATOM   3348   CA   ASP B  98    -3.049 -50.685 -46.188  1.00 29.78  BBBB
ATOM   3356   CA   VAL B  99    -0.296 -50.214 -43.660  1.00 26.75  BBBB
ATOM   3363   CA   VAL B 100     0.227 -50.613 -39.936  1.00 23.59  BBBB
ATOM   3370   CA   LEU B 101     2.214 -48.199 -37.797  1.00 21.59  BBBB
ATOM   3378   CA   GLY B 102     3.796 -49.357 -34.549  1.00 19.23  BBBB
ATOM   3382   CA   MET B 103     4.892 -46.597 -32.191  1.00 18.93  BBBB
ATOM   3390   CA   GLY B 104     6.275 -49.080 -29.686  1.00 21.89  BBBB
ATOM   3394   CA   GLY B 105     4.593 -50.905 -26.827  1.00 23.54  BBBB
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ATOM   3410   CA   VAL B 107     0.557 -54.694 -28.099  1.00 18.06  BBBB
ATOM   3417   CA   SER B 108     2.488 -53.892 -31.290  1.00 19.67  BBBB
ATOM   3423   CA   GLY B 109     4.251 -57.256 -31.023  1.00 20.03  BBBB
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ATOM   3507   CA   VAL B 122     4.743 -52.594 -41.083  1.00 22.03  BBBB
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ATOM   3529   CA   HIS B 125     8.814 -45.413 -34.981  1.00 21.42  BBBB
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ATOM   3618  CA   TRP B 137      12.753 -57.345 -32.424  1.00 22.06  BBBB
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ATOM   3667  CA   THR B 143       9.262 -52.595 -43.984  1.00 26.10  BBBB
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ATOM   3690  CA   MET B 146      12.338 -44.736 -37.993  1.00 23.15  BBBB
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ATOM   3845  CA   VAL B 167       6.746 -24.503 -29.440  1.00 25.91  BBBB
ATOM   3852  CA   LEU B 168       7.780 -25.002 -33.075  1.00 28.46  BBBB
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ATOM    4062  CA  ILE B 197     13.329 -34.168  -6.164  1.00 28.10      BBBB
ATOM    4070  CA  LEU B 198     13.069 -30.833  -8.003  1.00 26.58      BBBB
ATOM    4078  CA  ASN B 199     10.497 -29.447  -5.563  1.00 27.07      BBBB
ATOM    4086  CA  GLN B 200     12.955 -30.326  -2.794  1.00 30.10      BBBB
ATOM    4095  CA  THR B 201     16.215 -29.345  -4.474  1.00 27.34      BBBB
ATOM    4102  CA  MET B 202     15.567 -26.048  -6.268  1.00 23.68      BBBB
ATOM    4111  CA  PRO B 203     14.608 -23.963  -3.220  1.00 23.84      BBBB
ATOM    4117  CA  GLN B 204     18.033 -24.708  -1.684  1.00 26.34      BBBB
ATOM    4126  CA  VAL B 205     19.672 -24.033  -5.043  1.00 24.44      BBBB
ATOM    4133  CA  ALA B 206     17.980 -20.610  -5.013  1.00 22.84      BBBB
ATOM    4138  CA  ALA B 207     19.442 -19.857  -1.576  1.00 26.65      BBBB
ATOM    4143  CA  LYS B 208     22.915 -20.595  -2.919  1.00 28.31      BBBB
ATOM    4152  CA  LEU B 209     22.577 -18.640  -6.171  1.00 25.68      BBBB
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ATOM   4160  CA   GLY B 210     20.675 -15.628  -4.804  1.00 26.56 BBBB
ATOM   4164  CA   ASP B 211     20.370 -12.647  -7.190  1.00 28.28 BBBB
ATOM   4172  CA   SER B 212     22.098 -14.474 -10.067  1.00 25.73 BBBB
ATOM   4178  CA   VAL B 213     18.925 -16.308 -11.116  1.00 20.76 BBBB
ATOM   4185  CA   THR B 214     15.204 -15.726 -11.337  1.00 19.60 BBBB
ATOM   4192  CA   ILE B 215     13.076 -18.850 -11.169  1.00 18.75 BBBB
ATOM   4200  CA   TRP B 216      9.661 -19.973 -12.378  1.00 19.34 BBBB
ATOM   4214  CA   HIS B 217      9.015 -23.303 -10.680  1.00 21.06 BBBB
ATOM   4224  CA   GLN B 218      6.149 -25.594 -11.735  1.00 24.30 BBBB
ATOM   4233  CA   SER B 219      5.463 -27.800  -8.684  1.00 26.73 BBBB
ATOM   4239  CA   GLY B 220      2.855 -30.242  -9.961  1.00 30.53 BBBB
ATOM   4243  CA   LYS B 221     -0.657 -30.914  -8.628  1.00 35.12 BBBB
ATOM   4252  CA   GLY B 222     -1.195 -29.899  -5.011  1.00 35.34 BBBB
ATOM   4256  CA   SER B 223      2.451 -28.934  -4.418  1.00 33.98 BBBB
ATOM   4262  CA   GLN B 224      2.187 -25.208  -5.186  1.00 33.71 BBBB
ATOM   4271  CA   GLN B 225      1.823 -24.239  -1.519  1.00 32.32 BBBB
ATOM   4280  CA   SER B 226      4.701 -26.309  -0.122  1.00 28.30 BBBB
ATOM   4286  CA   VAL B 227      7.214 -25.247  -2.791  1.00 24.28 BBBB
ATOM   4293  CA   GLU B 228      6.178 -21.592  -2.387  1.00 27.23 BBBB
ATOM   4302  CA   GLN B 229      6.853 -22.046   1.329  1.00 28.38 BBBB
ATOM   4311  CA   ALA B 230     10.185 -23.754   0.682  1.00 26.18 BBBB
ATOM   4316  CA   TYR B 231     11.371 -20.766  -1.366  1.00 25.47 BBBB
ATOM   4328  CA   ALA B 232     10.342 -18.322   1.368  1.00 27.51 BBBB
ATOM   4333  CA   GLU B 233     12.145 -20.441   3.966  1.00 30.87 BBBB
ATOM   4342  CA   ALA B 234     15.215 -20.417   1.714  1.00 28.48 BBBB
ATOM   4347  CA   GLY B 235     15.033 -16.627   1.815  1.00 26.23 BBBB
ATOM   4351  CA   GLN B 236     14.121 -16.198  -1.870  1.00 25.53 BBBB
ATOM   4361  CA   PRO B 237     10.336 -15.587  -1.720  1.00 24.65 BBBB
ATOM   4367  CA   GLN B 238     10.277 -13.558  -4.945  1.00 24.29 BBBB
ATOM   4376  CA   HIS B 239     10.526 -16.608  -7.201  1.00 22.08 BBBB
ATOM   4386  CA   LYS B 240      7.375 -17.589  -9.105  1.00 23.26 BBBB
ATOM   4395  CA   VAL B 241      5.740 -20.911  -8.277  1.00 23.78 BBBB
ATOM   4402  CA   THR B 242      2.758 -22.301 -10.177  1.00 25.93 BBBB
ATOM   4409  CA   GLU B 243      0.999 -25.651  -9.837  1.00 27.03 BBBB
ATOM   4418  CA   PHE B 244      0.964 -26.068 -13.620  1.00 26.54 BBBB
ATOM   4429  CA   ILE B 245      1.932 -24.242 -16.802  1.00 28.48 BBBB
ATOM   4437  CA   ASP B 246     -0.754 -24.396 -19.457  1.00 36.00 BBBB
ATOM   4445  CA   ASP B 247      1.245 -22.392 -21.999  1.00 30.74 BBBB
ATOM   4453  CA   MET B 248      4.625 -24.136 -22.138  1.00 28.41 BBBB
ATOM   4461  CA   ALA B 249      5.512 -22.216 -25.290  1.00 24.67 BBBB
ATOM   4466  CA   ALA B 250      5.188 -18.933 -23.390  1.00 21.78 BBBB
ATOM   4471  CA   ALA B 251      7.301 -20.259 -20.501  1.00 20.85 BBBB
ATOM   4476  CA   TYR B 252      9.972 -21.616 -22.886  1.00 22.78 BBBB
ATOM   4488  CA   ALA B 253     10.131 -18.224 -24.636  1.00 23.54 BBBB
ATOM   4493  CA   TRP B 254     10.829 -16.534 -21.303  1.00 19.76 BBBB
ATOM   4507  CA   ALA B 255     13.399 -19.025 -20.003  1.00 19.51 BBBB
ATOM   4512  CA   ASP B 256     17.176 -19.026 -20.434  1.00 17.58 BBBB
ATOM   4520  CA   VAL B 257     17.535 -22.603 -19.194  1.00 18.53 BBBB
ATOM   4527  CA   VAL B 258     15.208 -25.456 -18.234  1.00 19.32 BBBB
ATOM   4534  CA   VAL B 259     15.581 -27.957 -15.374  1.00 19.85 BBBB
ATOM   4541  CA   CYS B 260     13.454 -31.055 -15.946  1.00 22.00 BBBB
ATOM   4546  N    ARG B 261     12.937 -33.397 -16.212  1.00 22.34 BBBB
ATOM   4547  CA   ARG B 261     13.170 -34.800 -16.515  1.00 23.75 BBBB
ATOM   4548  CB   ARG B 261     11.964 -35.663 -16.104  1.00 27.16 BBBB
ATOM   4549  CG   ARG B 261     11.376 -35.337 -14.738  1.00 31.82 BBBB
ATOM   4550  CD   ARG B 261     11.490 -36.473 -13.732  1.00 36.33 BBBB
ATOM   4551  NE   ARG B 261     12.865 -36.721 -13.323  1.00 38.48 BBBB
ATOM   4552  CZ   ARG B 261     13.218 -37.176 -12.125  1.00 37.25 BBBB
ATOM   4553  NH1  ARG B 261     12.295 -37.433 -11.204  1.00 38.46 BBBB
ATOM   4554  NH2  ARG B 261     14.499 -37.370 -11.848  1.00 36.79 BBBB
ATOM   4555  C    ARG B 261     13.351 -34.871 -18.032  1.00 23.98 BBBB
ATOM   4556  O    ARG B 261     13.117 -33.883 -18.746  1.00 22.44 BBBB
ATOM   4558  CA   SER B 262     13.975 -36.189 -19.948  1.00 23.18 BBBB
ATOM   4563  N    GLY B 263     11.850 -37.151 -20.619  1.00 22.74 BBBB
ATOM   4564  CA   GLY B 263     11.026 -38.079 -21.361  1.00 22.85 BBBB
ATOM   4565  C    GLY B 263     11.392 -37.793 -22.813  1.00 24.06 BBBB
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ATOM   4566  O    GLY B 263      11.908 -36.705 -23.121  1.00 22.75      BBBB
ATOM   4567  N    ALA B 264      11.130 -38.739 -23.708  1.00 23.37      BBBB
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ATOM   4581  CA   THR B 266      10.194 -33.557 -23.657  1.00 22.34      BBBB
ATOM   4588  CA   VAL B 267      13.730 -33.762 -25.023  1.00 21.11      BBBB
ATOM   4595  CA   SER B 268      12.411 -33.191 -28.567  1.00 21.96      BBBB
ATOM   4600  N    GLU B 269      10.928 -31.563 -27.557  1.00 21.64      BBBB
ATOM   4601  CA   GLU B 269      10.282 -30.272 -27.378  1.00 21.95      BBBB
ATOM   4602  CB   GLU B 269       9.213 -30.399 -26.292  1.00 24.72      BBBB
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ATOM   4605  OE1  GLU B 269       6.325 -29.915 -25.287  1.00 31.50      BBBB
ATOM   4606  OE2  GLU B 269       7.591 -29.057 -23.719  1.00 29.84      BBBB
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ATOM   4610  CA   ILE B 270      13.295 -28.698 -25.638  1.00 20.62      BBBB
ATOM   4618  CA   ALA B 271      15.440 -29.058 -28.776  1.00 22.45      BBBB
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ATOM   4628  CA   ALA B 273      12.361 -24.596 -28.407  1.00 21.97      BBBB
ATOM   4633  CA   GLY B 274      16.093 -24.023 -28.709  1.00 21.07      BBBB
ATOM   4637  CA   LEU B 275      16.666 -24.057 -24.966  1.00 19.78      BBBB
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ATOM   4665  CA   PHE B 279      18.266 -32.838 -17.392  1.00 21.59      BBBB
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ATOM   4720  CA   LYS B 285      17.767 -49.993 -14.571  1.00 45.34      BBBB
ATOM   4729  CA   ASP B 286      16.949 -49.299 -18.222  1.00 43.26      BBBB
ATOM   4737  CA   ARG B 287      17.951 -45.623 -17.883  1.00 36.28      BBBB
ATOM   4748  CA   GLN B 288      15.622 -44.804 -20.755  1.00 30.77      BBBB
ATOM   4756  N    GLN B 289      15.378 -42.554 -19.857  1.00 29.38      BBBB
ATOM   4757  CA   GLN B 289      15.474 -41.099 -19.904  1.00 29.46      BBBB
ATOM   4758  CB   GLN B 289      14.772 -40.472 -18.700  1.00 29.25      BBBB
ATOM   4759  CG   GLN B 289      13.265 -40.416 -18.883  1.00 29.32      BBBB
ATOM   4760  CD   GLN B 289      12.575 -39.585 -17.826  1.00 29.84      BBBB
ATOM   4761  OE1  GLN B 289      13.191 -38.728 -17.188  1.00 29.52      BBBB
ATOM   4762  NE2  GLN B 289      11.281 -39.821 -17.647  1.00 28.95      BBBB
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ATOM   4764  O    GLN B 289      17.173 -39.557 -20.585  1.00 29.12      BBBB
ATOM   4766  CA   TYR B 290      19.228 -40.984 -19.550  1.00 29.55      BBBB
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ATOM   4791  N    ASN B 292      17.658 -40.779 -23.508  1.00 25.52      BBBB
ATOM   4792  CA   ASN B 292      16.902 -39.784 -24.270  1.00 26.06      BBBB
ATOM   4793  CB   ASN B 292      15.484 -39.599 -23.709  1.00 24.78      BBBB
ATOM   4794  CG   ASN B 292      14.590 -40.811 -23.928  1.00 24.46      BBBB
ATOM   4795  OD1  ASN B 292      14.842 -41.641 -24.798  1.00 25.33      BBBB
ATOM   4796  ND2  ASN B 292      13.523 -40.900 -23.146  1.00 23.83      BBBB
ATOM   4797  C    ASN B 292      17.605 -38.427 -24.258  1.00 25.99      BBBB
ATOM   4798  O    ASN B 292      17.566 -37.687 -25.244  1.00 26.18      BBBB
ATOM   4799  N    ALA B 293      18.242 -38.105 -23.139  1.00 25.66      BBBB
ATOM   4800  CA   ALA B 293      18.926 -36.822 -22.979  1.00 25.69      BBBB
ATOM   4801  CB   ALA B 293      18.940 -36.422 -21.506  1.00 24.17      BBBB
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ATOM   4802  C   ALA B 293     20.346 -36.800 -23.521  1.00 25.67  BBBB
ATOM   4803  O   ALA B 293     20.855 -35.743 -23.902  1.00 25.52  BBBB
ATOM   4805  CA  LEU B 294     22.354 -38.088 -24.032  1.00 25.90  BBBB
ATOM   4814  CA  PRO B 295     21.998 -36.870 -27.635  1.00 26.15  BBBB
ATOM   4820  CA  LEU B 296     21.521 -33.265 -26.481  1.00 25.42  BBBB
ATOM   4828  CA  GLU B 297     24.354 -33.530 -23.953  1.00 28.78  BBBB
ATOM   4837  CA  LYS B 298     26.644 -34.947 -26.648  1.00 31.90  BBBB
ATOM   4846  CA  ALA B 299     25.773 -31.965 -28.847  1.00 30.38  BBBB
ATOM   4851  CA  GLY B 300     26.777 -29.635 -26.017  1.00 26.18  BBBB
ATOM   4855  CA  ALA B 301     23.214 -28.333 -25.638  1.00 22.50  BBBB
ATOM   4860  CA  ALA B 302     22.516 -29.770 -22.186  1.00 21.78  BBBB
ATOM   4865  CA  LYS B 303     23.979 -31.340 -19.048  1.00 25.86  BBBB
ATOM   4874  CA  ILE B 304     22.753 -34.598 -17.550  1.00 27.17  BBBB
ATOM   4882  CA  ILE B 305     22.843 -35.178 -13.813  1.00 29.01  BBBB
ATOM   4890  CA  GLU B 306     21.664 -38.702 -13.061  1.00 34.65  BBBB
ATOM   4899  CA  GLN B 307     20.377 -39.599  -9.613  1.00 40.54  BBBB
ATOM   4909  CA  PRO B 308     23.828 -40.891  -8.484  1.00 43.20  BBBB
ATOM   4915  CA  GLN B 309     25.247 -37.361  -8.787  1.00 43.46  BBBB
ATOM   4924  CA  LEU B 310     22.232 -35.166  -8.022  1.00 39.65  BBBB
ATOM   4932  CA  SER B 311     22.660 -32.714  -5.154  1.00 34.90  BBBB
ATOM   4938  CA  VAL B 312     21.990 -29.074  -4.341  1.00 31.50  BBBB
ATOM   4945  CA  ASP B 313     25.642 -28.202  -4.957  1.00 29.61  BBBB
ATOM   4953  CA  ALA B 314     25.782 -30.099  -8.254  1.00 26.47  BBBB
ATOM   4958  CA  VAL B 315     22.755 -28.215  -9.612  1.00 25.33  BBBB
ATOM   4965  CA  ALA B 316     23.888 -24.872  -8.199  1.00 27.13  BBBB
ATOM   4970  CA  ASN B 317     27.444 -25.246  -9.518  1.00 28.52  BBBB
ATOM   4978  CA  THR B 318     26.174 -26.371 -12.906  1.00 27.04  BBBB
ATOM   4985  CA  LEU B 319     23.883 -23.370 -13.357  1.00 25.21  BBBB
ATOM   4993  CA  ALA B 320     26.445 -20.931 -11.957  1.00 24.59  BBBB
ATOM   4998  CA  GLY B 321     28.934 -22.031 -14.591  1.00 24.34  BBBB
ATOM   5002  CA  TRP B 322     26.738 -21.007 -17.521  1.00 21.72  BBBB
ATOM   5016  CA  SER B 323     27.141 -17.404 -18.692  1.00 19.04  BBBB
ATOM   5022  CA  ARG B 324     24.725 -15.741 -21.112  1.00 18.09  BBBB
ATOM   5033  CA  GLU B 325     27.220 -16.368 -23.954  1.00 16.96  BBBB
ATOM   5042  CA  THR B 326     27.460 -20.055 -23.070  1.00 16.39  BBBB
ATOM   5049  CA  LEU B 327     23.659 -20.305 -22.780  1.00 17.27  BBBB
ATOM   5057  CA  LEU B 328     23.175 -18.745 -26.222  1.00 17.39  BBBB
ATOM   5065  CA  THR B 329     25.567 -21.335 -27.688  1.00 21.30  BBBB
ATOM   5072  CA  MET B 330     23.771 -24.153 -25.870  1.00 19.91  BBBB
ATOM   5080  CA  ALA B 331     20.412 -22.871 -27.098  1.00 18.49  BBBB
ATOM   5085  CA  GLU B 332     21.626 -22.827 -30.704  1.00 21.47  BBBB
ATOM   5094  CA  ARG B 333     23.040 -26.330 -30.408  1.00 23.77  BBBB
ATOM   5105  CA  ALA B 334     19.648 -27.420 -29.063  1.00 22.88  BBBB
ATOM   5110  CA  ARG B 335     17.795 -25.892 -32.002  1.00 23.54  BBBB
ATOM   5121  CA  ALA B 336     20.330 -27.477 -34.372  1.00 26.85  BBBB
ATOM   5126  CA  ALA B 337     19.740 -30.925 -32.865  1.00 30.89  BBBB
ATOM   5131  CA  SER B 338     16.008 -30.432 -33.408  1.00 32.41  BBBB
ATOM   5137  CA  ILE B 339     13.882 -31.941 -36.187  1.00 34.35  BBBB
ATOM   5146  CA  PRO B 340     10.733 -29.730 -36.600  1.00 34.94  BBBB
ATOM   5152  CA  ASP B 341      8.711 -31.820 -39.056  1.00 33.33  BBBB
ATOM   5160  CA  ALA B 342      8.875 -35.238 -37.411  1.00 29.09  BBBB
ATOM   5165  CA  THR B 343      5.115 -35.696 -37.744  1.00 28.55  BBBB
ATOM   5172  CA  GLU B 344      5.085 -34.933 -41.480  1.00 32.00  BBBB
ATOM   5181  CA  ARG B 345      8.138 -37.123 -42.067  1.00 31.44  BBBB
ATOM   5192  CA  VAL B 346      6.578 -40.151 -40.384  1.00 28.61  BBBB
ATOM   5199  CA  ALA B 347      3.249 -39.617 -42.137  1.00 28.96  BBBB
ATOM   5204  CA  ASN B 348      5.035 -39.286 -45.493  1.00 34.56  BBBB
ATOM   5212  CA  GLU B 349      6.954 -42.540 -44.956  1.00 34.86  BBBB
ATOM   5221  CA  VAL B 350      3.767 -44.306 -43.919  1.00 33.79  BBBB
ATOM   5228  CA  SER B 351      2.196 -42.946 -47.095  1.00 36.67  BBBB
ATOM   5234  CA  ARG B 352      5.114 -44.088 -49.251  1.00 40.03  BBBB
ATOM   5245  CA  VAL B 353      5.089 -47.587 -47.737  1.00 42.78  BBBB
ATOM   5252  CA  ALA B 354      1.336 -47.957 -48.212  1.00 47.24  BBBB
ATOM   5257  CA  ARG B 355      2.035 -46.964 -51.824  1.00 52.71  BBBB
ATOM   5268  CA  ALA B 356      4.453 -49.913 -51.809  1.00 54.93  BBBB
ATOM   5273  CA  LEU B 357      7.023 -47.522 -53.289  1.00 57.81  BBBB
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END

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TABLE 4 ATOMIC COORDINATES OF THE

DONOR NUCLEOTIDE BINDING SITE

REMARK   4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000

ATOM	1	N	LEU	B	187	13.695	-22.128	-15.588	1.00	15.92	N
ATOM	2	CA	LEU	B	187	12.361	-22.710	-15.604	1.00	16.75	C
ATOM	3	C	LEU	B	187	12.450	-24.146	-15.085	1.00	16.85	C
ATOM	4	O	LEU	B	187	13.115	-24.982	-15.688	1.00	17.18	O
ATOM	5	CB	LEU	B	187	11.813	-22.701	-17.035	1.00	16.85	C
ATOM	6	CG	LEU	B	187	10.445	-23.340	-17.276	1.00	18.63	C
ATOM	7	CD1	LEU	B	187	9.368	-22.478	-16.625	1.00	19.42	C
ATOM	8	CD2	LEU	B	187	10.198	-23.449	-18.783	1.00	19.11	C
ATOM	9	N	VAL	B	188	11.788	-24.426	-13.964	1.00	18.20	N
ATOM	10	CA	VAL	B	188	11.774	-25.775	-13.381	1.00	18.41	C
ATOM	11	C	VAL	B	188	10.434	-26.440	-13.739	1.00	19.88	C
ATOM	12	O	VAL	B	188	9.371	-25.967	-13.336	1.00	20.39	O
ATOM	13	CB	VAL	B	188	11.902	-25.714	-11.842	1.00	18.98	C
ATOM	14	CG1	VAL	B	188	12.088	-27.126	-11.270	1.00	18.50	C
ATOM	15	CG2.	VAL	B	188	13.061	-24.818	-11.449	1.00	18.83	C
ATOM	16	N	VAL	B	189	10.493	-27.532	-14.496	1.00	21.55	N
ATOM	17	CA	VAL	B	189	9.298	-28.234	-14.948	1.00	22.11	C
ATOM	18	C	VAL	B	189	9.191	-29.639	-14.351	1.00	23.90	C
ATOM	19	O	VAL	B	189	10.067	-30.478	-14.559	1.00	23.61	O
ATOM	20	CB	VAL	B	189	9.299	-28.342	-16.488	1.00	22.50	C
ATOM	21	CG1	VAL	B	189	8.009	-29.013	-16.981	1.00	22.70	C
ATOM	22	CG2	VAL	B	189	9.470	-26.943	-17.101	1.00	21.26	C
ATOM	23	N	GLY	B	190	8.111	-29.887	-13.615	1.00	25.60	N
ATOM	24	CA	GLY	B	190	7.914	-31.188	-12.994	1.00	27.28	C
ATOM	25	C	GLY	B	190	6.808	-32.026	-13.604	1.00	29.67	C
ATOM	26	O	GLY	B	190	6.668	-33.208	-13.283	1.00	29.86	O
ATOM	27	N	GLY	B	191	6.025	-31.430	-14.497	1.00	30.56	N
ATOM	28	CA	GLY	B	191	4.935	-32.163	-15.115	1.00	31.94	C
ATOM	29	C	GLY	B	191	3.676	-32.104	-14.269	1.00	33.11	C
ATOM	30	O	GLY	B	191	3.691	-31.556	-13.165	1.00	32.14	O
ATOM	31	N	ALA	B	195	7.761	-33.045	-9.938	1.00	33.54	N
ATOM	32	CA	ALA	B	195	8.977	-33.819	-9.709	1.00	33.12	C
ATOM	33	C	ALA	B	195	9.423	-33.590	-8.267	1.00	32.87	C
ATOM	34	O	ALA	B	195	9.955	-32.533	-7.923	1.00	31.47	O
ATOM	35	CB	ALA	B	195	10.073	-33.387	-10.679	1.00	33.17	C
ATOM	36	N	LEU	B	198	12.897	-32.223	-7.590	1.00	27.07	N
ATOM	37	CA	LEU	B	198	13.069	-30.833	-8.003	1.00	26.58	C
ATOM	38	C	LEU	B	198	12.388	-29.893	-7.006	1.00	26.41	C
ATOM	39	O	LEU	B	198	12.930	-28.835	-6.667	1.00	26.35	O
ATOM	40	CB	LEU	B	198	12.504	-30.616	-9.412	1.00	25.88	C
ATOM	41	CG	LEU	B	198	13.196	-31.408	-10.524	1.00	25.40	C
ATOM	42	CD1	LEU	B	198	12.625	-31.007	-11.874	1.00	26.54	C
ATOM	43	CD2	LEU	B	198	14.692	-31.146	-10.493	1.00	25.94	C
ATOM	44	N	TYR	B	252	8.723	-21.314	-22.184	1.00	21.27	N
ATOM	45	CA	TYR	B	252	9.972	-21.616	-22.886	1.00	22.78	C
ATOM	46	C	TYR	B	252	10.566	-20.354	-23.516	1.00	23.57	C
ATOM	47	O	TYR	B	252	11.784	-20.180	-23.550	1.00	23.91	O
ATOM	48	CB	TYR	B	252	9.726	-22.661	-23.980	1.00	21.62	C
ATOM	49	CG	TYR	B	252	9.662	-24.100	-23.505	1.00	23.34	C
ATOM	50	CD1	TYR	B	252	9.003	-25.065	-24.261	1.00	22.88	C
ATOM	51	CD2	TYR	B	252	10.288	-24.505	-22.319	1.00	22.30	C
ATOM	52	CE1	TYR	B	252	8.961	-26.392	-23.861	1.00	24.81	C
ATOM	53	CE2	TYR	B	252	10.253	-25.838	-21.912	1.00	23.56	C
ATOM	54	CZ	TYR	B	252	9.590	-26.772	-22.687	1.00	24.26	C
ATOM	55	OH	TYR	B	252	9.554	-28.088	-22.305	1.00	25.57	O
ATOM	56	N	VAL	B	258	16.263	-24.643	-18.818	1.00	18.74	N
ATOM	57	CA	VAL	B	258	15.208	-25.456	-18.234	1.00	19.32	C
ATOM	58	C	VAL	B	258	15.799	-26.585	-17.389	1.00	19.70	C

ATOM	59	O	VAL	B	258	16.808	-27.175	-17.758	1.00 18.96	O
ATOM	60	CB	VAL	B	258	14.328	-26.100	-19.337	1.00 19.89	C
ATOM	61	CG1	VAL	B	258	13.101	-26.754	-18.714	1.00 19.81	C
ATOM	62	CG2	VAL	B	258	13.907	-25.041	-20.364	1.00 21.59	C
ATOM	63	N	VAL	B	259	15.167	-26.861	-16.253	1.00 20.24	N
ATOM	64	CA	VAL	B	259	15.581	-27.957	-15.374	1.00 19.85	C
ATOM	65	C	VAL	B	259	14.382	-28.890	-15.371	1.00 20.02	C
ATOM	66	O	VAL	B	259	13.301	-28.500	-14.942	1.00 21.88	O
ATOM	67	CB	VAL	B	259	15.850	-27.483	-13.936	1.00 20.08	C
ATOM	68	CG1	VAL	B	259	16.222	-28.689	-13.059	1.00 20.22	C
ATOM	69	CG2	VAL	B	259	16.966	-26.453	-13.930	1.00 17.86	C
ATOM	70	N	CYS	B	260	14.562	-30.111	-15.867	1.00 21.70	N
ATOM	71	CA	CYS	B	260	13.454	-31.055	-15.946	1.00 22.00	C
ATOM	72	C	CYS	B	260	13.903	-32.478	-16.242	1.00 21.86	C
ATOM	73	O	CYS	B	260	15.087	-32.730	-16.496	1.00 21.34	O
ATOM	74	CB	CYS	B	260	12.494	-30.618	-17.057	1.00 22.77	C
ATOM	75	SG	CYS	B	260	13.297	-30.506	-18.711	1.00 22.15	S
ATOM	76	N	ARG	B	261	12.937	-33.397	-16.212	1.00 22.34	N
ATOM	77	CA	ARG	B	261	13.170	-34.800	-16.515	1.00 23.75	C
ATOM	78	C	ARG	B	261	13.351	-34.871	-18.032	1.00 23.98	C
ATOM	79	O	ARG	B	261	13.117	-33.883	-18.746	1.00 22.44	O
ATOM	80	CB	ARG	B	261	11.964	-35.663	-16.104	1.00 27.16	C
ATOM	81	CG	ARG	B	261	11.376	-35.337	-14.738	1.00 31.82	C
ATOM	82	CD	ARG	B	261	11.490	-36.473	-13.732	1.00 36.33	C
ATOM	83	NE	ARG	B	261	12.865	-36.721	-13.323	1.00 38.48	N
ATOM	84	CZ	ARG	B	261	13.218	-37.176	-12.125	1.00 37.25	C
ATOM	85	NH1	ARG	B	261	12.295	-37.433	-11.204	1.00 38.46	N
ATOM	86	NH2	ARG	B	261	14.499	-37.370	-11.848	1.00 36.79	N
ATOM	87	N	SER	B	262	13.740	-36.038	-18.527	1.00 22.00	N
ATOM	88	CA	SER	B	262	13.975	-36.189	-19.948	1.00 23.18	C
ATOM	89	C	SER	B	262	13.173	-37.263	-20.676	1.00 22.90	C
ATOM	90	O	SER	B	262	13.738	-38.179	-21.274	1.00 23.25	O
ATOM	91	CB	SER	B	262	15.481	-36.377	-20.203	1.00 24.45	C
ATOM	92	OG	SER	B	262	16.043	-37.326	-19.311	1.00 25.79	O
ATOM	93	N	GLY	B	263	11.850	-37.151	-20.619	1.00 22.74	N
ATOM	94	CA	GLY	B	263	11.026	-38.079	-21.361	1.00 22.85	C
ATOM	95	C	GLY	B	263	11.392	-37.793	-22.813	1.00 24.06	C
ATOM	96	O	GLY	B	263	11.908	-36.705	-23.121	1.00 22.75	O
ATOM	97	N	ALA	B	264	11.130	-38.739	-23.708	1.00 23.37	N
ATOM	98	CA	ALA	B	264	11.482	-38.564	-25.115	1.00 24.25	C
ATOM	99	C	ALA	B	264	10.843	-37.343	-25.783	1.00 24.29	C
ATOM	100	O	ALA	B	264	11.523	-36.572	-26.470	1.00 24.33	O
ATOM	101	CB	ALA	B	264	11.133	-39.829	-25.894	1.00 24.58	C
ATOM	102	N	LEU	B	265	9.541	-37.167	-25.596	1.00 24.44	N
ATOM	103	CA	LEU	B	265	8.846	-36.037	-26.205	1.00 24.66	C
ATOM	104	C	LEU	B	265	9.331	-34.717	-25.613	1.00 24.47	C
ATOM	105	O	LEU	B	265	9.374	-33.693	-26.301	1.00 23.85	O
ATOM	106	CB	LEU	B	265	7.332	-36.183	-26.011	1.00 25.33	C
ATOM	107	CG	LEU	B	265	6.760	-37.544	-26.426	1.00 27.97	C
ATOM	108	CD1	LEU	B	265	5.242	-37.541	-26.258	1.00 28.21	C
ATOM	109	CD2	LEU	B	265	7.146	-37.856	-27.878	1.00 27.40	C
ATOM	110	N	THR	B	266	9.702	-34.747	-24.338	1.00 22.12	N
ATOM	111	CA	THR	B	266	10.194	-33.557	-23.657	1.00 22.34	C
ATOM	112	C	THR	B	266	11.535	-33.117	-24.226	1.00 21.15	C
ATOM	113	O	THR	B	266	11.761	-31.926	-24.442	1.00 20.35	O
ATOM	114	CB	THR	B	266	10.348	-33.803	-22.140	1.00 22.35	C
ATOM	115	OG1	THR	B	266	9.061	-34.087	-21.583	1.00 24.46	O
ATOM	116	CG2	THR	B	266	10.945	-32.573	-21.444	1.00 24.00	C
ATOM	117	N	VAL	B	267	12.427	-34.075	-24.461	1.00 20.46	N
ATOM	118	CA	VAL	B	267	13.730	-33.762	-25.023	1.00 21.11	C
ATOM	119	C	VAL	B	267	13.548	-33.138	-26.416	1.00 21.34	C
ATOM	120	O	VAL	B	267	14.188	-32.135	-26.747	1.00 19.99	O
ATOM	121	CB	VAL	B	267	14.614	-35.039	-25.114	1.00 21.54	C
ATOM	122	CG1	VAL	B	267	15.903	-34.740	-25.865	1.00 20.72	C
ATOM	123	CG2	VAL	B	267	14.938	-35.541	-23.708	1.00 20.45	C
ATOM	124	N	SER	B	268	12.663	-33.717	-27.222	1.00 21.61	N

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ATOM    125  CA  SER B 268      12.411 -33.191 -28.567  1.00 21.96           C
ATOM    126  C   SER B 268      11.817 -31.790 -28.519  1.00 21.81           C
ATOM    127  O   SER B 268      12.158 -30.933 -29.336  1.00 22.60           O
ATOM    128  CB  SER B 268      11.474 -34.121 -29.344  1.00 21.57           C
ATOM    129  OG  SER B 268      12.141 -35.316 -29.721  1.00 24.06           O
ATOM    130  N   GLU B 269      10.928 -31.563 -27.557  1.00 21.64           N
ATOM    131  CA  GLU B 269      10.282 -30.272 -27.378  1.00 21.95           C
ATOM    132  C   GLU B 269      11.321 -29.214 -26.999  1.00 21.68           C
ATOM    133  O   GLU B 269      11.301 -28.095 -27.518  1.00 18.12           O
ATOM    134  CB  GLU B 269       9.213 -30.399 -26.292  1.00 24.72           C
ATOM    135  CG  GLU B 269       8.480 -29.128 -25.940  1.00 27.67           C
ATOM    136  CD  GLU B 269       7.385 -29.380 -24.908  1.00 30.05           C
ATOM    137  OE1 GLU B 269       6.325 -29.915 -25.287  1.00 31.50           O
ATOM    138  OE2 GLU B 269       7.591 -29.057 -23.719  1.00 29.84           O
ATOM    139  N   ILE B 270      12.224 -29.581 -26.092  1.00 19.43           N
ATOM    140  CA  ILE B 270      13.295 -28.698 -25.638  1.00 20.62           C
ATOM    141  C   ILE B 270      14.214 -28.314 -26.806  1.00 20.58           C
ATOM    142  O   ILE B 270      14.595 -27.151 -26.954  1.00 20.50           O
ATOM    143  CB  ILE B 270      14.157 -29.391 -24.533  1.00 20.30           C
ATOM    144  CG1 ILE B 270      13.337 -29.574 -23.254  1.00 21.32           C
ATOM    145  CG2 ILE B 270      15.415 -28.595 -24.266  1.00 19.17           C
ATOM    146  CD1 ILE B 270      12.926 -28.291 -22.583  1.00 23.40           C
ATOM    147  N   ALA B 277      19.316 -27.110 -21.396  1.00 17.01           N
ATOM    148  CA  ALA B 277      18.638 -27.807 -20.321  1.00 15.80           C
ATOM    149  C   ALA B 277      19.591 -28.526 -19.382  1.00 17.37           C
ATOM    150  O   ALA B 277      20.710 -28.891 -19.755  1.00 17.09           O
ATOM    151  CB  ALA B 277      17.641 -28.805 -20.895  1.00 17.01           C
ATOM    152  N   LEU B 278      19.147 -28.673 -18.138  1.00 17.14           N
ATOM    153  CA  LEU B 278      19.896 -29.429 -17.145  1.00 18.48           C
ATOM    154  C   LEU B 278      18.884 -30.535 -16.898  1.00 19.62           C
ATOM    155  O   LEU B 278      17.870 -30.330 -16.218  1.00 20.77           O
ATOM    156  CB  LEU B 278      20.140 -28.619 -15.869  1.00 19.19           C
ATOM    157  CG  LEU B 278      21.084 -29.308 -14.868  1.00 20.85           C
ATOM    158  CD1 LEU B 278      21.283 -28.411 -13.668  1.00 21.11           C
ATOM    159  CD2 LEU B 278      20.497 -30.647 -14.433  1.00 19.16           C
ATOM    160  N   PHE B 279      19.149 -31.691 -17.495  1.00 19.50           N
ATOM    161  CA  PHE B 279      18.266 -32.838 -17.392  1.00 21.59           C
ATOM    162  C   PHE B 279      18.525 -33.709 -16.167  1.00 22.86           C
ATOM    163  O   PHE B 279      19.671 -34.065 -15.871  1.00 23.32           O
ATOM    164  CB  PHE B 279      18.385 -33.700 -18.651  1.00 21.07           C
ATOM    165  CG  PHE B 279      17.740 -33.099 -19.876  1.00 19.35           C
ATOM    166  CD1 PHE B 279      18.481 -32.898 -21.035  1.00 19.42           C
ATOM    167  CD2 PHE B 279      16.379 -32.794 -19.888  1.00 18.16           C
ATOM    168  CE1 PHE B 279      17.874 -32.405 -22.203  1.00 19.06           C
ATOM    169  CE2 PHE B 279      15.759 -32.298 -21.052  1.00 17.65           C
ATOM    170  CZ  PHE B 279      16.515 -32.108 -22.208  1.00 15.61           C
ATOM    171  N   VAL B 280      17.445 -34.037 -15.461  1.00 23.88           N
ATOM    172  CA  VAL B 280      17.502 -34.902 -14.281  1.00 25.67           C
ATOM    173  C   VAL B 280      16.690 -36.136 -14.658  1.00 25.65           C
ATOM    174  O   VAL B 280      15.509 -36.239 -14.346  1.00 24.57           O
ATOM    175  CB  VAL B 280      16.883 -34.223 -13.048  1.00 26.89           C
ATOM    176  CG1 VAL B 280      16.954 -35.159 -11.847  1.00 28.12           C
ATOM    177  CG2 VAL B 280      17.631 -32.929 -12.742  1.00 27.70           C
ATOM    178  N   PRO B 281      17.324 -37.080 -15.370  1.00 27.08           N
ATOM    179  CA  PRO B 281      16.698 -38.320 -15.824  1.00 29.05           C
ATOM    180  C   PRO B 281      16.092 -39.121 -14.684  1.00 31.51           C
ATOM    181  O   PRO B 281      16.675 -39.223 -13.603  1.00 32.26           O
ATOM    182  CB  PRO B 281      17.851 -39.071 -16.492  1.00 29.44           C
ATOM    183  CG  PRO B 281      18.791 -37.992 -16.895  1.00 29.67           C
ATOM    184  CD  PRO B 281      18.750 -37.057 -15.726  1.00 27.31           C
ATOM    185  N   PHE B 282      14.908 -39.668 -14.923  1.00 33.83           N
ATOM    186  CA  PHE B 282      14.246 -40.496 -13.926  1.00 37.13           C
ATOM    187  C   PHE B 282      15.078 -41.776 -13.880  1.00 38.09           C
ATOM    188  O   PHE B 282      15.357 -42.373 -14.921  1.00 38.33           O
ATOM    189  CB  PHE B 282      12.818 -40.808 -14.372  1.00 38.38           C
ATOM    190  CG  PHE B 282      12.032 -41.606 -13.377  1.00 40.57           C
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ATOM	191	CD1	PHE B 282	11.720	-41.074	-12.130	1.00	41.80	C
ATOM	192	CD2	PHE B 282	11.590	-42.886	-13.689	1.00	41.65	C
ATOM	193	CE1	PHE B 282	10.975	-41.806	-11.209	1.00	42.03	C
ATOM	194	CE2	PHE B 282	10.843	-43.628	-12.773	1.00	42.49	C
ATOM	195	CZ	PHE B 282	10.536	-43.085	-11.532	1.00	41.74	C
ATOM	196	N	GLN B 288	16.212	-45.321	-19.533	1.00	30.94	N
ATOM	197	CA	GLN B 288	15.622	-44.804	-20.755	1.00	30.77	C
ATOM	198	C	GLN B 288	15.783	-43.291	-20.885	1.00	29.70	C
ATOM	199	O	GLN B 288	16.268	-42.801	-21.902	1.00	29.79	O
ATOM	200	CB	GLN B 288	14.143	-45.158	-20.810	1.00	30.59	C
ATOM	201	CG	GLN B 288	13.473	-44.772	-22.109	1.00	29.73	C
ATOM	202	CD	GLN B 288	11.981	-44.971	-22.044	1.00	28.04	C
ATOM	203	OE1	GLN B 288	11.294	-44.295	-21.279	1.00	29.59	O
ATOM	204	NE2	GLN B 288	11.468	-45.905	-22.838	1.00	26.98	N
ATOM	205	N	GLN B 289	15.378	-42.554	-19.857	1.00	29.38	N
ATOM	206	CA	GLN B 289	15.474	-41.099	-19.904	1.00	29.46	C
ATOM	207	C	GLN B 289	16.906	-40.613	-20.005	1.00	29.36	C
ATOM	208	O	GLN B 289	17.173	-39.557	-20.585	1.00	29.12	O
ATOM	209	CB	GLN B 289	14.772	-40.472	-18.700	1.00	29.25	C
ATOM	210	CG	GLN B 289	13.265	-40.416	-18.883	1.00	29.32	C
ATOM	211	CD	GLN B 289	12.575	-39.585	-17.826	1.00	29.84	C
ATOM	212	OE1	GLN B 289	13.191	-38.728	-17.188	1.00	29.52	O
ATOM	213	NE2	GLN B 289	11.281	-39.821	-17.647	1.00	28.95	N
ATOM	214	N	TYR B 290	17.835	-41.374	-19.442	1.00	28.95	N
ATOM	215	CA	TYR B 290	19.228	-40.984	-19.550	1.00	29.55	C
ATOM	216	C	TYR B 290	19.593	-41.042	-21.032	1.00	28.80	C
ATOM	217	O	TYR B 290	20.192	-40.113	-21.567	1.00	29.22	O
ATOM	218	CB	TYR B 290	20.136	-41.934	-18.768	1.00	31.40	C
ATOM	219	CG	TYR B 290	21.587	-41.780	-19.148	1.00	33.37	C
ATOM	220	CD1	TYR B 290	22.332	-40.682	-18.717	1.00	34.57	C
ATOM	221	CD2	TYR B 290	22.192	-42.684	-20.017	1.00	34.90	C
ATOM	222	CE1	TYR B 290	23.644	-40.490	-19.148	1.00	35.97	C
ATOM	223	CE2	TYR B 290	23.497	-42.500	-20.453	1.00	36.03	C
ATOM	224	CZ	TYR B 290	24.214	-41.402	-20.019	1.00	36.29	C
ATOM	225	OH	TYR B 290	25.499	-41.215	-20.475	1.00	39.44	O
ATOM	226	N	ASN B 292	17.658	-40.779	-23.508	1.00	25.52	N
ATOM	227	CA	ASN B 292	16.902	-39.784	-24.270	1.00	26.06	C
ATOM	228	C	ASN B 292	17.605	-38.427	-24.258	1.00	25.99	C
ATOM	229	O	ASN B 292	17.566	-37.687	-25.244	1.00	26.18	O
ATOM	230	CB	ASN B 292	15.484	-39.599	-23.709	1.00	24.78	C
ATOM	231	CG	ASN B 292	14.590	-40.811	-23.928	1.00	24.46	C
ATOM	232	OD1	ASN B 292	14.842	-41.641	-24.798	1.00	25.33	O
ATOM	233	ND2	ASN B 292	13.523	-40.900	-23.146	1.00	23.83	N
ATOM	234	N	ALA B 293	18.242	-38.105	-23.139	1.00	25.66	N
ATOM	235	CA	ALA B 293	18.926	-36.822	-22.979	1.00	25.69	C
ATOM	236	C	ALA B 293	20.346	-36.800	-23.521	1.00	25.67	C
ATOM	237	O	ALA B 293	20.855	-35.743	-23.902	1.00	25.52	O
ATOM	238	CB	ALA B 293	18.940	-36.422	-21.506	1.00	24.17	C
ATOM	239	N	LEU B 296	21.375	-34.703	-26.688	1.00	25.66	N
ATOM	240	CA	LEU B 296	21.521	-33.265	-26.481	1.00	25.42	C
ATOM	241	C	LEU B 296	22.784	-32.935	-25.688	1.00	26.07	C
ATOM	242	O	LEU B 296	23.435	-31.917	-25.944	1.00	25.26	O
ATOM	243	CB	LEU B 296	20.283	-32.685	-25.779	1.00	24.45	C
ATOM	244	CG	LEU B 296	19.066	-32.458	-26.679	1.00	25.59	C
ATOM	245	CD1	LEU B 296	17.968	-31.718	-25.911	1.00	23.56	C
ATOM	246	CD2	LEU B 296	19.496	-31.630	-27.893	1.00	25.87	C
ATOM	247	N	ALA B 302	23.066	-29.504	-23.507	1.00	20.94	N
ATOM	248	CA	ALA B 302	22.516	-29.770	-22.186	1.00	21.78	C
ATOM	249	C	ALA B 302	23.503	-30.507	-21.288	1.00	22.69	C
ATOM	250	O	ALA B 302	24.561	-30.948	-21.739	1.00	22.25	O
ATOM	251	CB	ALA B 302	21.243	-30.595	-22.327	1.00	20.10	C
ATOM	252	N	LYS B 303	23.156	-30.613	-20.009	1.00	24.62	N
ATOM	253	CA	LYS B 303	23.979	-31.340	-19.048	1.00	25.86	C
ATOM	254	C	LYS B 303	23.083	-32.319	-18.302	1.00	26.41	C
ATOM	255	O	LYS B 303	22.015	-31.948	-17.802	1.00	25.76	O
ATOM	256	CB	LYS B 303	24.632	-30.401	-18.036	1.00	27.85	C

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ATOM    257  CG   LYS B 303      25.466 -31.146 -16.986  1.00 29.37       C
ATOM    258  CD   LYS B 303      26.150 -30.186 -16.025  1.00 32.41       C
ATOM    259  CE   LYS B 303      27.083 -30.912 -15.056  1.00 33.22       C
ATOM    260  NZ   LYS B 303      27.827 -29.952 -14.181  1.00 33.62       N
ATOM    261  N    ILE B 304      23.520 -33.570 -18.234  1.00 25.65       N
ATOM    262  CA   ILE B 304      22.753 -34.598 -17.550  1.00 27.17       C
ATOM    263  C    ILE B 304      23.308 -34.855 -16.160  1.00 27.00       C
ATOM    264  O    ILE B 304      24.511 -35.012 -15.986  1.00 27.46       O
ATOM    265  CB   ILE B 304      22.786 -35.946 -18.316  1.00 27.06       C
ATOM    266  CG1  ILE B 304      22.242 -35.769 -19.733  1.00 27.61       C
ATOM    267  CG2  ILE B 304      21.977 -36.996 -17.555  1.00 28.49       C
ATOM    268  CD1  ILE B 304      22.380 -37.009 -20.599  1.00 27.05       C
ATOM    269  N    ILE B 305      22.428 -34.869 -15.168  1.00 27.22       N
ATOM    270  CA   ILE B 305      22.843 -35.178 -13.813  1.00 29.01       C
ATOM    271  C    ILE B 305      21.934 -36.302 -13.351  1.00 29.64       C
ATOM    272  O    ILE B 305      20.806 -36.067 -12.932  1.00 29.25       O
ATOM    273  CB   ILE B 305      22.713 -33.977 -12.858  1.00 28.91       C
ATOM    274  CG1  ILE B 305      23.660 -32.855 -13.299  1.00 29.51       C
ATOM    275  CG2  ILE B 305      23.063 -34.416 -11.432  1.00 30.98       C
ATOM    276  CD1  ILE B 305      23.674 -31.653 -12.367  1.00 29.43       C
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TABLE 5 ATOMIC COORDINATES OF ACCEPTOR BINDING SITE

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REMARK   4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   MET B  12    -0.734 -48.902 -33.817  1.00 23.68       N
ATOM      2  CA  MET B  12    -0.523 -49.707 -32.613  1.00 24.54       C
ATOM      3  C   MET B  12     0.361 -48.840 -31.720  1.00 25.31       C
ATOM      4  O   MET B  12     1.546 -48.645 -32.006  1.00 23.88       O
ATOM      5  CB  MET B  12     0.192 -51.019 -32.971  1.00 24.28       C
ATOM      6  CG  MET B  12    -0.402 -51.726 -34.188  1.00 25.19       C
ATOM      7  SD  MET B  12     0.399 -53.284 -34.669  1.00 26.54       S
ATOM      8  CE  MET B  12     1.990 -52.691 -35.289  1.00 22.99       C
ATOM      9  N   ALA B  13    -0.224 -48.292 -30.657  1.00 27.08       N
ATOM     10  CA  ALA B  13     0.508 -47.410 -29.752  1.00 29.43       C
ATOM     11  C   ALA B  13    -0.239 -47.192 -28.436  1.00 31.80       C
ATOM     12  O   ALA B  13    -1.143 -46.350 -28.352  1.00 32.16       O
ATOM     13  CB  ALA B  13     0.747 -46.074 -30.429  1.00 28.82       C
ATOM     14  N   GLY B  14     0.150 -47.934 -27.405  1.00 32.46       N
ATOM     15  CA  GLY B  14    -0.513 -47.804 -26.120  1.00 33.82       C
ATOM     16  C   GLY B  14    -0.107 -46.595 -25.299  1.00 34.82       C
ATOM     17  O   GLY B  14     0.975 -46.040 -25.479  1.00 35.47       O
ATOM     18  N   GLY B  15    -0.986 -46.188 -24.385  1.00 35.56       N
ATOM     19  CA  GLY B  15    -0.700 -45.047 -23.536  1.00 36.08       C
ATOM     20  C   GLY B  15     0.539 -45.254 -22.683  1.00 36.84       C
ATOM     21  O   GLY B  15     1.293 -44.311 -22.426  1.00 36.03       O
ATOM     22  N   THR B  16     0.755 -46.488 -22.240  1.00 36.65       N
ATOM     23  CA  THR B  16     1.920 -46.787 -21.421  1.00 38.51       C
ATOM     24  C   THR B  16     3.158 -46.497 -22.264  1.00 38.35       C
ATOM     25  O   THR B  16     3.191 -46.798 -23.460  1.00 39.90       O
ATOM     26  CB  THR B  16     1.926 -48.258 -20.974  1.00 38.51       C
ATOM     27  OG1 THR B  16     0.686 -48.558 -20.321  1.00 38.39       O
ATOM     28  CG2 THR B  16     3.075 -48.518 -20.005  1.00 39.11       C
ATOM     29  N   GLY B  17     4.168 -45.897 -21.649  1.00 37.68       N
ATOM     30  CA  GLY B  17     5.367 -45.567 -22.392  1.00 36.57       C
ATOM     31  C   GLY B  17     5.161 -44.303 -23.211  1.00 35.56       C
ATOM     32  O   GLY B  17     6.079 -43.843 -23.890  1.00 35.03       O
ATOM     33  N   GLY B  18     3.949 -43.752 -23.150  1.00 33.83       N
ATOM     34  CA  GLY B  18     3.631 -42.529 -23.872  1.00 33.48       C
ATOM     35  C   GLY B  18     3.825 -42.593 -25.378  1.00 33.12       C
ATOM     36  O   GLY B  18     4.345 -41.650 -25.984  1.00 35.38       O
ATOM     37  N   HIS B  19     3.416 -43.699 -25.988  1.00 30.26       N
ATOM     38  CA  HIS B  19     3.548 -43.865 -27.435  1.00 28.22       C
ATOM     39  C   HIS B  19     2.280 -43.370 -28.144  1.00 27.91       C
ATOM     40  O   HIS B  19     2.300 -43.049 -29.337  1.00 26.91       O
ATOM     41  CB  HIS B  19     3.772 -45.349 -27.779  1.00 25.81       C
ATOM     42  CG  HIS B  19     4.957 -45.966 -27.094  1.00 25.35       C
ATOM     43  ND1 HIS B  19     4.845 -47.025 -26.217  1.00 24.57       N
ATOM     44  CD2 HIS B  19     6.281 -45.694 -27.184  1.00 24.18       C
ATOM     45  CE1 HIS B  19     6.046 -47.380 -25.798  1.00 23.08       C
ATOM     46  NE2 HIS B  19     6.936 -46.589 -26.369  1.00 25.51       N
ATOM     47  N   VAL B  20     1.180 -43.310 -27.402  1.00 27.65       N
ATOM     48  CA  VAL B  20    -0.098 -42.894 -27.965  1.00 27.77       C
ATOM     49  C   VAL B  20    -0.140 -41.452 -28.470  1.00 27.57       C
ATOM     50  O   VAL B  20    -0.771 -41.172 -29.486  1.00 27.12       O
ATOM     51  CB  VAL B  20    -1.248 -43.080 -26.942  1.00 28.57       C
ATOM     52  CG1 VAL B  20    -1.082 -42.114 -25.787  1.00 30.03       C
ATOM     53  CG2 VAL B  20    -2.602 -42.873 -27.631  1.00 26.82       C
ATOM     54  N   LEU B  40    -5.323 -50.004 -32.549  1.00 25.21       N
ATOM     55  CA  LEU B  40    -5.200 -51.364 -32.026  1.00 24.71       C
ATOM     56  C   LEU B  40    -4.535 -51.235 -30.655  1.00 23.33       C
ATOM     57  O   LEU B  40    -3.387 -50.824 -30.563  1.00 23.43       O
ATOM     58  CB  LEU B  40    -4.326 -52.221 -32.952  1.00 25.21       C
ATOM     59  CG  LEU B  40    -4.416 -53.754 -32.868  1.00 26.95       C
ATOM     60  CD1 LEU B  40    -3.037 -54.334 -32.571  1.00 27.63       C
ATOM     61  CD2 LEU B  40    -5.421 -54.179 -31.817  1.00 26.69       C
ATOM     62  N   GLU B  47    -4.976 -45.941 -23.678  1.00 32.85       N
ATOM     63  CA  GLU B  47    -5.458 -45.655 -25.029  1.00 31.79       C
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ATOM	64	C	GLU	B	47	-6.938	-46.017	-25.191	1.00	31.81	C
ATOM	65	O	GLU	B	47	-7.626	-45.476	-26.055	1.00	31.31	O
ATOM	66	CB	GLU	B	47	-4.624	-46.402	-26.080	1.00	30.62	C
ATOM	67	CG	GLU	B	47	-4.755	-47.922	-26.051	1.00	29.85	C
ATOM	68	CD	GLU	B	47	-3.793	-48.597	-25.082	1.00	29.78	C
ATOM	69	OE1	GLU	B	47	-3.188	-47.895	-24.247	1.00	28.76	O
ATOM	70	OE2	GLU	B	47	-3.649	-49.840	-25.156	1.00	29.01	O
ATOM	71	N	ILE	B	63	-3.428	-59.342	-24.313	1.00	30.07	N
ATOM	72	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00	31.38	C
ATOM	73	C	ILE	B	63	-1.623	-59.981	-22.775	1.00	33.08	C
ATOM	74	O	ILE	B	63	-0.444	-59.872	-22.430	1.00	33.21	O
ATOM	75	CB	ILE	B	63	-1.081	-58.745	-24.883	1.00	30.06	C
ATOM	76	CG1	ILE	B	63	-1.143	-57.411	-24.137	1.00	29.94	C
ATOM	77	CG2	ILE	B	63	-1.442	-58.567	-26.353	1.00	30.41	C
ATOM	78	CD1	ILE	B	63	-0.128	-56.384	-24.632	1.00	29.62	C
ATOM	79	N	ARG	B	67	2.953	-59.185	-21.440	1.00	31.54	N
ATOM	80	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90	C
ATOM	81	C	ARG	B	67	5.071	-58.142	-20.713	1.00	29.99	C
ATOM	82	O	ARG	B	67	5.294	-59.034	-19.889	1.00	28.67	O
ATOM	83	CB	ARG	B	67	2.888	-56.984	-20.363	1.00	32.28	C
ATOM	84	CG	ARG	B	67	1.540	-56.576	-20.913	1.00	34.65	C
ATOM	85	CD	ARG	B	67	0.926	-55.440	-20.097	1.00	36.69	C
ATOM	86	NE	ARG	B	67	-0.259	-54.889	-20.748	1.00	38.28	N
ATOM	87	CZ	ARG	B	67	-1.425	-55.519	-20.853	1.00	39.05	C
ATOM	88	NH1	ARG	B	67	-1.583	-56.734	-20.341	1.00	39.61	N
ATOM	89	NH2	ARG	B	67	-2.434	-54.935	-21.487	1.00	39.52	N
ATOM	90	N	GLY	B	68	6.014	-57.321	-21.165	1.00	27.75	N
ATOM	91	CA	GLY	B	68	7.380	-57.427	-20.685	1.00	26.79	C
ATOM	92	C	GLY	B	68	8.166	-58.579	-21.280	1.00	25.41	C
ATOM	93	O	GLY	B	68	9.326	-58.779	-20.943	1.00	26.04	O
ATOM	94	N	GLY	B	102	3.556	-48.986	-35.936	1.00	20.96	N
ATOM	95	CA	GLY	B	102	3.796	-49.357	-34.549	1.00	19.23	C
ATOM	96	C	GLY	B	102	4.655	-48.282	-33.918	1.00	18.45	C
ATOM	97	O	GLY	B	102	5.765	-48.016	-34.381	1.00	18.70	O
ATOM	98	N	MET	B	103	4.155	-47.660	-32.857	1.00	18.01	N
ATOM	99	CA	MET	B	103	4.892	-46.597	-32.191	1.00	18.93	C
ATOM	100	C	MET	B	103	5.612	-47.128	-30.957	1.00	18.98	C
ATOM	101	O	MET	B	103	6.134	-46.357	-30.158	1.00	17.96	O
ATOM	102	CB	MET	B	103	3.928	-45.477	-31.781	1.00	20.02	C
ATOM	103	CG	MET	B	103	3.121	-44.888	-32.944	1.00	21.61	C
ATOM	104	SD	MET	B	103	4.212	-44.135	-34.157	1.00	23.45	S
ATOM	105	CE	MET	B	103	4.718	-42.680	-33.271	1.00	21.40	C
ATOM	106	N	GLY	B	104	5.640	-48.450	-30.827	1.00	21.56	N
ATOM	107	CA	GLY	B	104	6.275	-49.080	-29.686	1.00	21.89	C
ATOM	108	C	GLY	B	104	5.192	-49.614	-28.764	1.00	23.28	C
ATOM	109	O	GLY	B	104	4.009	-49.353	-28.980	1.00	22.50	O
ATOM	110	N	GLY	B	105	5.583	-50.364	-27.741	1.00	23.01	N
ATOM	111	CA	GLY	B	105	4.593	-50.905	-26.827	1.00	23.54	C
ATOM	112	C	GLY	B	105	4.358	-52.380	-27.078	1.00	23.17	C
ATOM	113	O	GLY	B	105	4.449	-52.844	-28.214	1.00	22.69	O
ATOM	114	N	TYR	B	106	4.018	-53.118	-26.026	1.00	22.87	N
ATOM	115	CA	TYR	B	106	3.818	-54.554	-26.159	1.00	22.37	C
ATOM	116	C	TYR	B	106	2.719	-55.018	-27.100	1.00	20.52	C
ATOM	117	O	TYR	B	106	2.867	-56.052	-27.746	1.00	20.50	O
ATOM	118	CB	TYR	B	106	3.632	-55.181	-24.774	1.00	25.08	C
ATOM	119	CG	TYR	B	106	4.864	-55.008	-23.929	1.00	28.19	C
ATOM	120	CD1	TYR	B	106	4.869	-54.153	-22.830	1.00	31.96	C
ATOM	121	CD2	TYR	B	106	6.058	-55.631	-24.282	1.00	31.27	C
ATOM	122	CE1	TYR	B	106	6.043	-53.915	-22.108	1.00	33.13	C
ATOM	123	CE2	TYR	B	106	7.234	-55.400	-23.569	1.00	32.27	C
ATOM	124	CZ	TYR	B	106	7.219	-54.541	-22.487	1.00	33.19	C
ATOM	125	OH	TYR	B	106	8.388	-54.291	-21.802	1.00	35.95	O
ATOM	126	N	VAL	B	107	1.628	-54.270	-27.205	1.00	19.06	N
ATOM	127	CA	VAL	B	107	0.557	-54.694	-28.099	1.00	18.06	C
ATOM	128	C	VAL	B	107	1.015	-54.743	-29.559	1.00	17.45	C
ATOM	129	O	VAL	B	107	0.502	-55.536	-30.346	1.00	16.99	O

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ATOM    130  CB   VAL B 107     -0.690 -53.774 -27.978  1.00 20.95      C
ATOM    131  CG1  VAL B 107     -0.407 -52.407 -28.589  1.00 21.39      C
ATOM    132  CG2  VAL B 107     -1.879 -54.433 -28.658  1.00 21.30      C
ATOM    133  N    SER B 108      1.991 -53.916 -29.918  1.00 17.96      N
ATOM    134  CA   SER B 108      2.488 -53.892 -31.290  1.00 19.67      C
ATOM    135  C    SER B 108      3.197 -55.187 -31.694  1.00 20.38      C
ATOM    136  O    SER B 108      3.385 -55.449 -32.884  1.00 21.25      O
ATOM    137  CB   SER B 108      3.424 -52.691 -31.508  1.00 19.56      C
ATOM    138  OG   SER B 108      4.666 -52.824 -30.837  1.00 19.63      O
ATOM    139  N    GLY B 109      3.595 -55.995 -30.710  1.00 19.59      N
ATOM    140  CA   GLY B 109      4.251 -57.256 -31.023  1.00 20.03      C
ATOM    141  C    GLY B 109      3.311 -58.170 -31.792  1.00 19.61      C
ATOM    142  O    GLY B 109      3.579 -58.517 -32.940  1.00 19.24      O
ATOM    143  N    PRO B 110      2.206 -58.606 -31.173  1.00 19.20      N
ATOM    144  CA   PRO B 110      1.251 -59.478 -31.855  1.00 18.99      C
ATOM    145  C    PRO B 110      0.651 -58.761 -33.075  1.00 19.22      C
ATOM    146  O    PRO B 110      0.406 -59.371 -34.116  1.00 17.13      O
ATOM    147  CB   PRO B 110      0.198 -59.737 -30.778  1.00 20.41      C
ATOM    148  CG   PRO B 110      0.998 -59.720 -29.515  1.00 19.81      C
ATOM    149  CD   PRO B 110      1.914 -58.528 -29.729  1.00 19.94      C
ATOM    150  N    HIS B 125      8.182 -46.638 -35.447  1.00 21.40      N
ATOM    151  CA   HIS B 125      8.814 -45.413 -34.981  1.00 21.42      C
ATOM    152  C    HIS B 125      9.196 -45.642 -33.519  1.00 21.70      C
ATOM    153  O    HIS B 125      8.378 -46.117 -32.725  1.00 19.81      O
ATOM    154  CB   HIS B 125      7.858 -44.218 -35.067  1.00 21.57      C
ATOM    155  CG   HIS B 125      8.432 -42.948 -34.511  1.00 23.73      C
ATOM    156  ND1  HIS B 125      9.274 -42.127 -35.236  1.00 26.23      N
ATOM    157  CD2  HIS B 125      8.300 -42.368 -33.295  1.00 22.15      C
ATOM    158  CE1  HIS B 125      9.631 -41.095 -34.490  1.00 24.20      C
ATOM    159  NE2  HIS B 125      9.054 -41.218 -33.307  1.00 26.07      N
ATOM    160  N    GLU B 126     10.444 -45.332 -33.186  1.00 21.20      N
ATOM    161  CA   GLU B 126     10.947 -45.452 -31.817  1.00 22.15      C
ATOM    162  C    GLU B 126     11.205 -44.027 -31.326  1.00 21.93      C
ATOM    163  O    GLU B 126     12.016 -43.300 -31.908  1.00 21.33      O
ATOM    164  CB   GLU B 126     12.252 -46.246 -31.790  1.00 21.99      C
ATOM    165  CG   GLU B 126     12.958 -46.206 -30.439  1.00 22.04      C
ATOM    166  CD   GLU B 126     12.119 -46.824 -29.338  1.00 21.43      C
ATOM    167  OE1  GLU B 126     11.767 -48.014 -29.471  1.00 21.92      O
ATOM    168  OE2  GLU B 126     11.807 -46.124 -28.349  1.00 21.08      O
ATOM    169  N    GLN B 127     10.520 -43.624 -30.259  1.00 22.62      N
ATOM    170  CA   GLN B 127     10.682 -42.270 -29.735  1.00 22.81      C
ATOM    171  C    GLN B 127     11.874 -42.087 -28.809  1.00 22.39      C
ATOM    172  O    GLN B 127     12.399 -40.976 -28.682  1.00 22.43      O
ATOM    173  CB   GLN B 127      9.414 -41.814 -28.989  1.00 23.56      C
ATOM    174  CG   GLN B 127      8.147 -41.783 -29.830  1.00 24.46      C
ATOM    175  CD   GLN B 127      7.312 -43.041 -29.687  1.00 25.85      C
ATOM    176  OE1  GLN B 127      6.842 -43.366 -28.591  1.00 23.78      O
ATOM    177  NE2  GLN B 127      7.119 -43.758 -30.797  1.00 24.91      N
ATOM    178  N    ASN B 128     12.314 -43.173 -28.177  1.00 22.35      N
ATOM    179  CA   ASN B 128     13.406 -43.097 -27.216  1.00 22.96      C
ATOM    180  C    ASN B 128     14.824 -43.314 -27.742  1.00 23.87      C
ATOM    181  O    ASN B 128     15.026 -43.856 -28.830  1.00 24.05      O
ATOM    182  CB   ASN B 128     13.136 -44.080 -26.064  1.00 22.85      C
ATOM    183  CG   ASN B 128     11.742 -43.919 -25.474  1.00 23.25      C
ATOM    184  OD1  ASN B 128     10.804 -44.632 -25.848  1.00 26.04      O
ATOM    185  ND2  ASN B 128     11.597 -42.975 -24.556  1.00 22.68      N
ATOM    186  N    GLY B 132     12.851 -49.814 -27.506  1.00 24.52      N
ATOM    187  CA   GLY B 132     12.007 -50.532 -26.568  1.00 24.05      C
ATOM    188  C    GLY B 132     12.150 -52.019 -26.831  1.00 23.35      C
ATOM    189  O    GLY B 132     12.582 -52.419 -27.904  1.00 22.89      O
ATOM    190  N    LEU B 133     11.788 -52.846 -25.860  1.00 23.38      N
ATOM    191  CA   LEU B 133     11.903 -54.293 -26.020  1.00 24.54      C
ATOM    192  C    LEU B 133     11.209 -54.833 -27.276  1.00 22.84      C
ATOM    193  O    LEU B 133     11.784 -55.619 -28.027  1.00 21.86      O
ATOM    194  CB   LEU B 133     11.328 -54.996 -24.786  1.00 25.48      C
ATOM    195  CG   LEU B 133     11.388 -56.527 -24.780  1.00 27.50      C
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ATOM    196  CD1 LEU B 133     12.840 -56.984 -24.866  1.00 28.69      C
ATOM    197  CD2 LEU B 133     10.735 -57.059 -23.509  1.00 28.04      C
ATOM    198  N   THR B 134      9.975 -54.401 -27.499  1.00 21.72      N
ATOM    199  CA  THR B 134      9.202 -54.860 -28.639  1.00 21.22      C
ATOM    200  C   THR B 134      9.693 -54.326 -29.986  1.00 20.62      C
ATOM    201  O   THR B 134      9.843 -55.091 -30.932  1.00 20.33      O
ATOM    202  CB  THR B 134      7.716 -54.509 -28.449  1.00 20.99      C
ATOM    203  OG1 THR B 134      7.257 -55.075 -27.210  1.00 20.94      O
ATOM    204  CG2 THR B 134      6.872 -55.073 -29.600  1.00 20.64      C
ATOM    205  N   ASN B 135      9.932 -53.021 -30.075  1.00 21.24      N
ATOM    206  CA  ASN B 135     10.407 -52.419 -31.324  1.00 20.50      C
ATOM    207  C   ASN B 135     11.724 -53.064 -31.767  1.00 20.78      C
ATOM    208  O   ASN B 135     11.945 -53.290 -32.953  1.00 20.41      O
ATOM    209  CB  ASN B 135     10.637 -50.911 -31.142  1.00 19.58      C
ATOM    210  CG  ASN B 135      9.457 -50.058 -31.597  1.00 19.93      C
ATOM    211  OD1 ASN B 135      9.454 -48.837 -31.390  1.00 21.78      O
ATOM    212  ND2 ASN B 135      8.467 -50.677 -32.219  1.00 17.21      N
ATOM    213  N   LEU B 138     10.741 -56.381 -33.386  1.00 21.61      N
ATOM    214  CA  LEU B 138      9.744 -56.188 -34.431  1.00 23.15      C
ATOM    215  C   LEU B 138     10.384 -55.558 -35.676  1.00 23.07      C
ATOM    216  O   LEU B 138      9.958 -55.801 -36.809  1.00 22.68      O
ATOM    217  CB  LEU B 138      8.618 -55.305 -33.886  1.00 23.87      C
ATOM    218  CG  LEU B 138      7.312 -55.155 -34.664  1.00 26.48      C
ATOM    219  CD1 LEU B 138      6.672 -56.508 -34.915  1.00 25.34      C
ATOM    220  CD2 LEU B 138      6.383 -54.267 -33.851  1.00 25.90      C
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TABLE 6 ATOMIC COORDINATES OF MEMBRANE ASSOCIATION SITE

REMARK	4	1MUR	COMPLIES	WITH	FORMAT V. 2.0, 11-MAY-2000					
ATOM	1	N	MET	B	12	-0.734	-48.902	-33.817	1.00	23.68	N
ATOM	2	CA	MET	B	12	-0.523	-49.707	-32.613	1.00	24.54	C
ATOM	3	C	MET	B	12	0.361	-48.840	-31.720	1.00	25.31	C
ATOM	4	O	MET	B	12	1.546	-48.645	-32.006	1.00	23.88	O
ATOM	5	CB	MET	B	12	0.192	-51.019	-32.971	1.00	24.28	C
ATOM	6	CG	MET	B	12	-0.402	-51.726	-34.188	1.00	25.19	C
ATOM	7	SD	MET	B	12	0.399	-53.284	-34.669	1.00	26.54	S
ATOM	8	CE	MET	B	12	1.990	-52.691	-35.289	1.00	22.99	C
ATOM	9	N	LEU	B	40	-5.323	-50.004	-32.549	1.00	25.21	N
ATOM	10	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00	24.71	C
ATOM	11	C	LEU	B	40	-4.535	-51.235	-30.655	1.00	23.33	C
ATOM	12	O	LEU	B	40	-3.387	-50.824	-30.563	1.00	23.43	O
ATOM	13	CB	LEU	B	40	-4.326	-52.221	-32.952	1.00	25.21	C
ATOM	14	CG	LEU	B	40	-4.416	-53.754	-32.868	1.00	26.95	C
ATOM	15	CD1	LEU	B	40	-3.037	-54.334	-32.571	1.00	27.63	C
ATOM	16	CD2	LEU	B	40	-5.421	-54.179	-31.817	1.00	26.69	C
ATOM	17	N	ILE	B	61	-7.271	-56.229	-28.295	1.00	29.38	N
ATOM	18	CA	ILE	B	61	-6.832	-57.616	-28.269	1.00	28.55	C
ATOM	19	C	ILE	B	61	-6.344	-57.855	-26.848	1.00	29.13	C
ATOM	20	O	ILE	B	61	-6.124	-56.906	-26.091	1.00	28.80	O
ATOM	21	CB	ILE	B	61	-5.674	-57.923	-29.258	1.00	28.48	C
ATOM	22	CG1	ILE	B	61	-4.422	-57.126	-28.892	1.00	26.70	C
ATOM	23	CG2	ILE	B	61	-6.123	-57.650	-30.694	1.00	27.65	C
ATOM	24	CD1	ILE	B	61	-3.177	-57.615	-29.638	1.00	27.03	C
ATOM	25	N	ARG	B	62	-6.186	-59.116	-26.473	1.00	29.38	N
ATOM	26	CA	ARG	B	62	-5.709	-59.416	-25.133	1.00	30.76	C
ATOM	27	C	ARG	B	62	-4.274	-59.923	-25.156	1.00	29.32	C
ATOM	28	O	ARG	B	62	-3.933	-60.809	-25.934	1.00	28.65	O
ATOM	29	CB	ARG	B	62	-6.630	-60.447	-24.461	1.00	32.36	C
ATOM	30	CG	ARG	B	62	-6.130	-60.955	-23.114	1.00	35.99	C
ATOM	31	CD	ARG	B	62	-5.438	-59.859	-22.311	1.00	37.86	C
ATOM	32	NE	ARG	B	62	-6.297	-58.718	-22.004	1.00	40.01	N
ATOM	33	CZ	ARG	B	62	-5.840	-57.504	-21.711	1.00	39.09	C
ATOM	34	NH1	ARG	B	62	-4.536	-57.275	-21.690	1.00	39.24	N
ATOM	35	NH2	ARG	B	62	-6.686	-56.518	-21.439	1.00	40.03	N
ATOM	36	N	ILE	B	63	-3.428	-59.342	-24.313	1.00	30.07	N
ATOM	37	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00	31.38	C
ATOM	38	C	ILE	B	63	-1.623	-59.981	-22.775	1.00	33.08	C
ATOM	39	O	ILE	B	63	-0.444	-59.872	-22.430	1.00	33.21	O
ATOM	40	CB	ILE	B	63	-1.081	-58.745	-24.883	1.00	30.06	C
ATOM	41	CG1	ILE	B	63	-1.143	-57.411	-24.137	1.00	29.94	C
ATOM	42	CG2	ILE	B	63	-1.442	-58.567	-26.353	1.00	30.41	C
ATOM	43	CD1	ILE	B	63	-0.128	-56.384	-24.632	1.00	29.62	C
ATOM	44	N	SER	B	64	-2.603	-60.284	-21.927	1.00	35.38	N
ATOM	45	CA	SER	B	64	-2.356	-60.520	-20.505	1.00	37.51	C
ATOM	46	C	SER	B	64	-1.326	-61.622	-20.311	1.00	37.32	C
ATOM	47	O	SER	B	64	-1.411	-62.682	-20.933	1.00	37.86	O
ATOM	48	CB	SER	B	64	-3.652	-60.912	-19.792	1.00	38.82	C
ATOM	49	OG	SER	B	64	-4.558	-59.823	-19.750	1.00	42.88	O
ATOM	50	N	GLY	B	65	-0.356	-61.370	-19.441	1.00	37.81	N
ATOM	51	CA	GLY	B	65	0.679	-62.355	-19.199	1.00	37.13	C
ATOM	52	C	GLY	B	65	1.798	-62.283	-20.226	1.00	36.76	C
ATOM	53	O	GLY	B	65	2.858	-62.889	-20.038	1.00	37.57	O
ATOM	54	N	LEU	B	66	1.577	-61.539	-21.307	1.00	34.63	N
ATOM	55	CA	LEU	B	66	2.591	-61.413	-22.355	1.00	33.17	C
ATOM	56	C	LEU	B	66	3.414	-60.133	-22.246	1.00	32.72	C
ATOM	57	O	LEU	B	66	4.451	-60.002	-22.893	1.00	33.13	O
ATOM	58	CB	LEU	B	66	1.936	-61.470	-23.735	1.00	32.08	C
ATOM	59	CG	LEU	B	66	1.162	-62.747	-24.061	1.00	32.52	C
ATOM	60	CD1	LEU	B	66	0.563	-62.626	-25.445	1.00	31.38	C

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ATOM	61	CD2	LEU	B	66	2.093	-63.957	-23.984	1.00	31.67	C
ATOM	62	N	ARG	B	67	2.953	-59.185	-21.440	1.00	31.54	N
ATOM	63	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90	C
ATOM	64	C	ARG	B	67	5.071	-58.142	-20.713	1.00	29.99	C
ATOM	65	O	ARG	B	67	5.294	-59.034	-19.889	1.00	28.67	O
ATOM	66	CB	ARG	B	67	2.888	-56.984	-20.363	1.00	32.28	C
ATOM	67	CG	ARG	B	67	1.540	-56.576	-20.913	1.00	34.65	C
ATOM	68	CD	ARG	B	67	0.926	-55.440	-20.097	1.00	36.69	C
ATOM	69	NE	ARG	B	67	-0.259	-54.889	-20.748	1.00	38.28	N
ATOM	70	CZ	ARG	B	67	-1.425	-55.519	-20.853	1.00	39.05	C
ATOM	71	NH1	ARG	B	67	-1.583	-56.734	-20.341	1.00	39.61	N
ATOM	72	NH2	ARG	B	67	-2.434	-54.935	-21.487	1.00	39.52	N
ATOM	73	N	GLY	B	68	6.014	-57.321	-21.165	1.00	27.75	N
ATOM	74	CA	GLY	B	68	7.380	-57.427	-20.685	1.00	26.79	C
ATOM	75	C	GLY	B	68	8.166	-58.579	-21.280	1.00	25.41	C
ATOM	76	O	GLY	B	68	9.326	-58.779	-20.943	1.00	26.04	O
ATOM	77	N	LYS	B	69	7.546	-59.342	-22.170	1.00	24.55	N
ATOM	78	CA	LYS	B	69	8.238	-60.463	-22.796	1.00	23.93	C
ATOM	79	C	LYS	B	69	8.825	-60.062	-24.142	1.00	23.32	C
ATOM	80	O	LYS	B	69	8.151	-59.404	-24.944	1.00	21.96	O
ATOM	81	CB	LYS	B	69	7.284	-61.641	-23.033	1.00	24.12	C
ATOM	82	CG	LYS	B	69	6.757	-62.360	-21.794	1.00	25.08	C
ATOM	83	CD	LYS	B	69	5.887	-63.553	-22.224	1.00	25.44	C
ATOM	84	CE	LYS	B	69	5.357	-64.358	-21.035	1.00	28.31	C
ATOM	85	NZ	LYS	B	69	6.468	-64.877	-20.175	1.00	29.71	N
ATOM	86	N	GLY	B	70	10.075	-60.470	-24.374	1.00	22.48	N
ATOM	87	CA	GLY	B	70	10.755	-60.229	-25.636	1.00	22.26	C
ATOM	88	C	GLY	B	70	10.308	-61.337	-26.588	1.00	22.17	C
ATOM	89	O	GLY	B	70	9.512	-62.183	-26.195	1.00	21.62	O
ATOM	90	N	ILE	B	71	10.819	-61.373	-27.814	1.00	21.85	N
ATOM	91	CA	ILE	B	71	10.357	-62.386	-28.762	1.00	23.55	C
ATOM	92	C	ILE	B	71	10.616	-63.840	-28.359	1.00	23.88	C
ATOM	93	O	ILE	B	71	9.775	-64.707	-28.592	1.00	21.66	O
ATOM	94	CB	ILE	B	71	10.926	-62.142	-30.181	1.00	23.52	C
ATOM	95	CG1	ILE	B	71	10.264	-63.096	-31.182	1.00	24.18	C
ATOM	96	CG2	ILE	B	71	12.435	-62.375	-30.192	1.00	25.96	C
ATOM	97	CD1	ILE	B	71	8.745	-62.981	-31.263	1.00	25.73	C
ATOM	98	N	LYS	B	72	11.764	-64.119	-27.751	1.00	23.82	N
ATOM	99	CA	LYS	B	72	12.038	-65.491	-27.343	1.00	24.92	C
ATOM	100	C	LYS	B	72	11.068	-65.925	-26.245	1.00	23.73	C
ATOM	101	O	LYS	B	72	10.592	-67.062	-26.245	1.00	24.08	O
ATOM	102	CB	LYS	B	72	13.491	-65.634	-26.875	1.00	26.86	C
ATOM	103	CG	LYS	B	72	14.496	-65.590	-28.019	1.00	31.29	C
ATOM	104	CD	LYS	B	72	15.925	-65.791	-27.518	1.00	36.00	C
ATOM	105	CE	LYS	B	72	16.926	-65.816	-28.671	1.00	38.82	C
ATOM	106	NZ	LYS	B	72	18.342	-65.957	-28.192	1.00	41.21	N
ATOM	107	N	ALA	B	73	10.765	-65.016	-25.322	1.00	21.62	N
ATOM	108	CA	ALA	B	73	9.839	-65.306	-24.233	1.00	21.18	C
ATOM	109	C	ALA	B	73	8.412	-65.454	-24.771	1.00	20.36	C
ATOM	110	O	ALA	B	73	7.619	-66.250	-24.267	1.00	18.97	O
ATOM	111	CB	ALA	B	73	9.895	-64.196	-23.187	1.00	22.25	C
ATOM	112	N	LEU	B	74	8.076	-64.673	-25.791	1.00	20.23	N
ATOM	113	CA	LEU	B	74	6.745	-64.762	-26.387	1.00	19.36	C
ATOM	114	C	LEU	B	74	6.549	-66.110	-27.069	1.00	19.37	C
ATOM	115	O	LEU	B	74	5.539	-66.779	-26.863	1.00	20.01	O
ATOM	116	CB	LEU	B	74	6.540	-63.643	-27.417	1.00	18.42	C
ATOM	117	CG	LEU	B	74	6.422	-62.208	-26.884	1.00	18.80	C
ATOM	118	CD1	LEU	B	74	6.473	-61.197	-28.039	1.00	19.86	C
ATOM	119	CD2	LEU	B	74	5.109	-62.071	-26.104	1.00	19.45	C
ATOM	120	N	ILE	B	75	7.520	-66.507	-27.883	1.00	20.59	N
ATOM	121	CA	ILE	B	75	7.434	-67.768	-28.601	1.00	21.18	C
ATOM	122	C	ILE	B	75	7.488	-68.942	-27.624	1.00	21.20	C
ATOM	123	O	ILE	B	75	7.125	-70.063	-27.979	1.00	21.59	O
ATOM	124	CB	ILE	B	75	8.571	-67.896	-29.641	1.00	22.95	C
ATOM	125	CG1	ILE	B	75	8.598	-66.657	-30.540	1.00	26.82	C
ATOM	126	CG2	ILE	B	75	8.334	-69.108	-30.527	1.00	25.38	C

ATOM	127	CD1	ILE	B	75	7.304	-66.442	-31.327	1.00	28.48	C
ATOM	128	N	ALA	B	76	7.940	-68.680	-26.399	1.00	20.49	N
ATOM	129	CA	ALA	B	76	7.996	-69.726	-25.374	1.00	21.72	C
ATOM	130	C	ALA	B	76	6.624	-69.904	-24.732	1.00	21.54	C
ATOM	131	O	ALA	B	76	6.441	-70.778	-23.875	1.00	20.75	O
ATOM	132	CB	ALA	B	76	9.026	-69.372	-24.305	1.00	21.92	C
ATOM	133	N	ALA	B	77	5.668	-69.066	-25.145	1.00	20.61	N
ATOM	134	CA	ALA	B	77	4.289	-69.121	-24.655	1.00	21.07	C
ATOM	135	C	ALA	B	77	3.383	-69.298	-25.881	1.00	21.69	C
ATOM	136	O	ALA	B	77	2.567	-68.430	-26.199	1.00	21.93	O
ATOM	137	CB	ALA	B	77	3.937	-67.830	-23.924	1.00	20.10	C
ATOM	138	N	PRO	B	78	3.507	-70.446	-26.564	1.00	22.38	N
ATOM	139	CA	PRO	B	78	2.772	-70.846	-27.771	1.00	20.95	C
ATOM	140	C	PRO	B	78	1.278	-70.535	-27.813	1.00	21.19	C
ATOM	141	O	PRO	B	78	0.789	-69.939	-28.776	1.00	19.68	O
ATOM	142	CB	PRO	B	78	3.027	-72.350	-27.861	1.00	22.21	C
ATOM	143	CG	PRO	B	78	4.288	-72.547	-27.117	1.00	24.07	C
ATOM	144	CD	PRO	B	78	4.211	-71.603	-25.976	1.00	21.89	C
ATOM	145	N	LEU	B	79	0.544	-70.961	-26.790	1.00	21.21	N
ATOM	146	CA	LEU	B	79	-0.896	-70.728	-26.783	1.00	21.32	C
ATOM	147	C	LEU	B	79	-1.275	-69.263	-26.707	1.00	21.17	C
ATOM	148	O	LEU	B	79	-2.125	-68.800	-27.481	1.00	20.44	O
ATOM	149	CB	LEU	B	79	-1.569	-71.476	-25.630	1.00	20.99	C
ATOM	150	CG	LEU	B	79	-1.397	-72.988	-25.617	1.00	22.40	C
ATOM	151	CD1	LEU	B	79	-2.504	-73.619	-24.772	1.00	22.01	C
ATOM	152	CD2	LEU	B	79	-1.438	-73.521	-27.021	1.00	23.82	C
ATOM	153	N	ARG	B	80	-0.656	-68.529	-25.788	1.00	20.91	N
ATOM	154	CA	ARG	B	80	-0.980	-67.115	-25.637	1.00	21.30	C
ATOM	155	C	ARG	B	80	-0.526	-66.233	-26.790	1.00	21.29	C
ATOM	156	O	ARG	B	80	-1.278	-65.355	-27.223	1.00	21.47	O
ATOM	157	CB	ARG	B	80	-0.444	-66.583	-24.312	1.00	22.12	C
ATOM	158	CG	ARG	B	80	-1.286	-67.051	-23.118	1.00	24.03	C
ATOM	159	CD	ARG	B	80	-0.610	-66.738	-21.807	1.00	23.42	C
ATOM	160	NE	ARG	B	80	0.581	-67.556	-21.610	1.00	24.59	N
ATOM	161	CZ	ARG	B	80	1.466	-67.351	-20.642	1.00	26.08	C
ATOM	162	NH1	ARG	B	80	1.290	-66.349	-19.787	1.00	26.92	N
ATOM	163	NH2	ARG	B	80	2.514	-68.152	-20.519	1.00	27.22	N
ATOM	164	N	ILE	B	81	0.683	-66.448	-27.303	1.00	19.29	N
ATOM	165	CA	ILE	B	81	1.113	-65.621	-28.421	1.00	19.47	C
ATOM	166	C	ILE	B	81	0.256	-65.937	-29.654	1.00	18.99	C
ATOM	167	O	ILE	B	81	-0.149	-65.028	-30.378	1.00	19.38	O
ATOM	168	CB	ILE	B	81	2.639	-65.793	-28.730	1.00	17.92	C
ATOM	169	CG1	ILE	B	81	3.067	-64.753	-29.769	1.00	18.63	C
ATOM	170	CG2	ILE	B	81	2.949	-67.200	-29.206	1.00	17.33	C
ATOM	171	CD1	ILE	B	81	2.746	-63.318	-29.346	1.00	17.46	C
ATOM	172	N	PHE	B	82	-0.056	-67.211	-29.880	1.00	19.39	N
ATOM	173	CA	PHE	B	82	-0.875	-67.582	-31.038	1.00	19.15	C
ATOM	174	C	PHE	B	82	-2.250	-66.931	-30.959	1.00	19.94	C
ATOM	175	O	PHE	B	82	-2.777	-66.444	-31.970	1.00	19.64	O
ATOM	176	CB	PHE	B	82	-1.057	-69.103	-31.136	1.00	19.27	C
ATOM	177	CG	PHE	B	82	-1.811	-69.548	-32.368	1.00	19.87	C
ATOM	178	CD1	PHE	B	82	-1.180	-69.602	-33.603	1.00	20.87	C
ATOM	179	CD2	PHE	B	82	-3.154	-69.898	-32.289	1.00	21.11	C
ATOM	180	CE1	PHE	B	82	-1.872	-70.002	-34.753	1.00	21.20	C
ATOM	181	CE2	PHE	B	82	-3.857	-70.297	-33.429	1.00	22.26	C
ATOM	182	CZ	PHE	B	82	-3.212	-70.349	-34.663	1.00	22.14	C
ATOM	183	N	ASN	B	83	-2.832	-66.923	-29.764	1.00	19.29	N
ATOM	184	CA	ASN	B	83	-4.150	-66.332	-29.577	1.00	20.90	C
ATOM	185	C	ASN	B	83	-4.178	-64.821	-29.812	1.00	20.83	C
ATOM	186	O	ASN	B	83	-5.086	-64.316	-30.472	1.00	21.92	O
ATOM	187	CB	ASN	B	83	-4.693	-66.641	-28.178	1.00	20.55	C
ATOM	188	CG	ASN	B	83	-6.158	-66.244	-28.028	1.00	22.79	C
ATOM	189	OD1	ASN	B	83	-6.505	-65.374	-27.229	1.00	25.14	O
ATOM	190	ND2	ASN	B	83	-7.018	-66.877	-28.807	1.00	20.47	N
ATOM	191	N	ALA	B	84	-3.203	-64.092	-29.275	1.00	19.74	N
ATOM	192	CA	ALA	B	84	-3.177	-62.647	-29.484	1.00	19.30	C

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ATOM    193  C    ALA B  84     -2.967 -62.380 -30.981  1.00 19.94      C
ATOM    194  O    ALA B  84     -3.561 -61.459 -31.552  1.00 19.69      O
ATOM    195  CB   ALA B  84     -2.060 -62.008 -28.662  1.00 18.59      C
ATOM    196  N    TRP B  85     -2.118 -63.197 -31.603  1.00 19.77      N
ATOM    197  CA   TRP B  85     -1.820 -63.111 -33.032  1.00 20.56      C
ATOM    198  C    TRP B  85     -3.090 -63.354 -33.865  1.00 21.76      C
ATOM    199  O    TRP B  85     -3.339 -62.658 -34.859  1.00 20.40      O
ATOM    200  CB   TRP B  85     -0.754 -64.148 -33.396  1.00 21.46      C
ATOM    201  CG   TRP B  85     -0.365 -64.167 -34.856  1.00 23.00      C
ATOM    202  CD1  TRP B  85      0.301 -63.189 -35.548  1.00 23.17      C
ATOM    203  CD2  TRP B  85     -0.588 -65.232 -35.785  1.00 23.69      C
ATOM    204  NE1  TRP B  85      0.509 -63.585 -36.848  1.00 24.28      N
ATOM    205  CE2  TRP B  85     -0.024 -64.835 -37.022  1.00 24.14      C
ATOM    206  CE3  TRP B  85     -1.206 -66.486 -35.693  1.00 24.79      C
ATOM    207  CZ2  TRP B  85     -0.060 -65.650 -38.160  1.00 24.90      C
ATOM    208  CZ3  TRP B  85     -1.243 -67.299 -36.827  1.00 25.45      C
ATOM    209  CH2  TRP B  85     -0.671 -66.875 -38.045  1.00 25.15      C
ATOM    210  N    ARG B  86     -3.885 -64.346 -33.467  1.00 22.03      N
ATOM    211  CA   ARG B  86     -5.140 -64.660 -34.166  1.00 23.28      C
ATOM    212  C    ARG B  86     -6.151 -63.517 -34.007  1.00 22.98      C
ATOM    213  O    ARG B  86     -6.890 -63.195 -34.942  1.00 21.37      O
ATOM    214  CB   ARG B  86     -5.754 -65.965 -33.623  1.00 24.72      C
ATOM    215  CG   ARG B  86     -4.999 -67.236 -34.021  1.00 27.21      C
ATOM    216  CD   ARG B  86     -5.368 -67.725 -35.418  1.00 29.60      C
ATOM    217  NE   ARG B  86     -6.626 -68.477 -35.422  1.00 31.45      N
ATOM    218  CZ   ARG B  86     -7.185 -69.004 -36.508  1.00 31.37      C
ATOM    219  NH1  ARG B  86     -6.607 -68.862 -37.696  1.00 32.19      N
ATOM    220  NH2  ARG B  86     -8.314 -69.694 -36.405  1.00 31.39      N
ATOM    221  N    GLN B  87     -6.190 -62.916 -32.821  1.00 22.90      N
ATOM    222  CA   GLN B  87     -7.101 -61.802 -32.567  1.00 24.07      C
ATOM    223  C    GLN B  87     -6.738 -60.618 -33.457  1.00 23.85      C
ATOM    224  O    GLN B  87     -7.613 -60.012 -34.077  1.00 24.02      O
ATOM    225  CB   GLN B  87     -7.046 -61.382 -31.097  1.00 24.33      C
ATOM    226  CG   GLN B  87     -7.873 -62.280 -30.187  1.00 27.24      C
ATOM    227  CD   GLN B  87     -7.720 -61.943 -28.723  1.00 28.81      C
ATOM    228  OE1  GLN B  87     -8.567 -62.296 -27.908  1.00 33.25      O
ATOM    229  NE2  GLN B  87     -6.632 -61.275 -28.375  1.00 29.95      N
ATOM    230  N    ALA B  88     -5.449 -60.293 -33.521  1.00 23.39      N
ATOM    231  CA   ALA B  88     -4.996 -59.183 -34.355  1.00 23.78      C
ATOM    232  C    ALA B  88     -5.257 -59.485 -35.831  1.00 24.73      C
ATOM    233  O    ALA B  88     -5.655 -58.595 -36.592  1.00 24.72      O
ATOM    234  CB   ALA B  88     -3.508 -58.909 -34.116  1.00 23.33      C
ATOM    235  N    ARG B  89     -5.038 -60.735 -36.244  1.00 24.26      N
ATOM    236  CA   ARG B  89     -5.285 -61.111 -37.636  1.00 24.94      C
ATOM    237  C    ARG B  89     -6.752 -60.909 -38.013  1.00 25.29      C
ATOM    238  O    ARG B  89     -7.056 -60.420 -39.104  1.00 24.27      O
ATOM    239  CB   ARG B  89     -4.904 -62.575 -37.893  1.00 25.14      C
ATOM    240  CG   ARG B  89     -3.461 -62.774 -38.353  1.00 24.54      C
ATOM    241  CD   ARG B  89     -3.142 -64.253 -38.510  1.00 25.50      C
ATOM    242  NE   ARG B  89     -3.809 -64.901 -39.641  1.00 24.93      N
ATOM    243  CZ   ARG B  89     -3.329 -64.930 -40.882  1.00 25.90      C
ATOM    244  NH1  ARG B  89     -2.178 -64.336 -41.170  1.00 25.98      N
ATOM    245  NH2  ARG B  89     -3.979 -65.596 -41.831  1.00 26.36      N
ATOM    246  N    GLY B 105      5.583 -50.364 -27.741  1.00 23.01      N
ATOM    247  CA   GLY B 105      4.593 -50.905 -26.827  1.00 23.54      C
ATOM    248  C    GLY B 105      4.358 -52.380 -27.078  1.00 23.17      C
ATOM    249  O    GLY B 105      4.449 -52.844 -28.214  1.00 22.69      O
ATOM    250  N    TYR B 106      4.018 -53.118 -26.026  1.00 22.87      N
ATOM    251  CA   TYR B 106      3.818 -54.554 -26.159  1.00 22.37      C
ATOM    252  C    TYR B 106      2.719 -55.018 -27.100  1.00 20.52      C
ATOM    253  O    TYR B 106      2.867 -56.052 -27.746  1.00 20.50      O
ATOM    254  CB   TYR B 106      3.632 -55.181 -24.774  1.00 25.08      C
ATOM    255  CG   TYR B 106      4.864 -55.008 -23.929  1.00 28.19      C
ATOM    256  CD1  TYR B 106      4.869 -54.153 -22.830  1.00 31.96      C
ATOM    257  CD2  TYR B 106      6.058 -55.631 -24.282  1.00 31.27      C
ATOM    258  CE1  TYR B 106      6.043 -53.915 -22.108  1.00 33.13      C
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ATOM    259  CE2 TYR B 106       7.234 -55.400 -23.569  1.00 32.27       C
ATOM    260  CZ  TYR B 106       7.219 -54.541 -22.487  1.00 33.19       C
ATOM    261  OH  TYR B 106       8.388 -54.291 -21.802  1.00 35.95       O
ATOM    262  N   VAL B 107       1.628 -54.270 -27.205  1.00 19.06       N
ATOM    263  CA  VAL B 107       0.557 -54.694 -28.099  1.00 18.06       C
ATOM    264  C   VAL B 107       1.015 -54.743 -29.559  1.00 17.45       C
ATOM    265  O   VAL B 107       0.502 -55.536 -30.346  1.00 16.99       O
ATOM    266  CB  VAL B 107      -0.690 -53.774 -27.978  1.00 20.95       C
ATOM    267  CG1 VAL B 107      -0.407 -52.407 -28.589  1.00 21.39       C
ATOM    268  CG2 VAL B 107      -1.879 -54.433 -28.658  1.00 21.30       C
ATOM    269  N   SER B 108       1.991 -53.916 -29.918  1.00 17.96       N
ATOM    270  CA  SER B 108       2.488 -53.892 -31.290  1.00 19.67       C
ATOM    271  C   SER B 108       3.197 -55.187 -31.694  1.00 20.38       C
ATOM    272  O   SER B 108       3.385 -55.449 -32.884  1.00 21.25       O
ATOM    273  CB  SER B 108       3.424 -52.691 -31.508  1.00 19.56       C
ATOM    274  OG  SER B 108       4.666 -52.824 -30.837  1.00 19.63       O
ATOM    275  N   GLY B 109       3.595 -55.995 -30.710  1.00 19.59       N
ATOM    276  CA  GLY B 109       4.251 -57.256 -31.023  1.00 20.03       C
ATOM    277  C   GLY B 109       3.311 -58.170 -31.792  1.00 19.61       C
ATOM    278  O   GLY B 109       3.579 -58.517 -32.940  1.00 19.24       O
ATOM    279  N   PRO B 110       2.206 -58.606 -31.173  1.00 19.20       N
ATOM    280  CA  PRO B 110       1.251 -59.478 -31.855  1.00 18.99       C
ATOM    281  C   PRO B 110       0.651 -58.761 -33.075  1.00 19.22       C
ATOM    282  O   PRO B 110       0.406 -59.371 -34.116  1.00 17.13       O
ATOM    283  CB  PRO B 110       0.198 -59.737 -30.778  1.00 20.41       C
ATOM    284  CG  PRO B 110       0.998 -59.720 -29.515  1.00 19.81       C
ATOM    285  CD  PRO B 110       1.914 -58.528 -29.729  1.00 19.94       C
ATOM    286  N   GLY B 111       0.407 -57.462 -32.927  1.00 19.03       N
ATOM    287  CA  GLY B 111      -0.160 -56.702 -34.025  1.00 19.60       C
ATOM    288  C   GLY B 111       0.764 -56.714 -35.226  1.00 19.59       C
ATOM    289  O   GLY B 111       0.330 -56.979 -36.339  1.00 21.10       O
ATOM    290  N   GLY B 112       2.043 -56.429 -34.995  1.00 19.78       N
ATOM    291  CA  GLY B 112       3.014 -56.417 -36.074  1.00 19.97       C
ATOM    292  C   GLY B 112       3.147 -57.783 -36.724  1.00 20.43       C
ATOM    293  O   GLY B 112       3.233 -57.896 -37.949  1.00 19.94       O
ATOM    294  N   LEU B 113       3.167 -58.828 -35.903  1.00 19.26       N
ATOM    295  CA  LEU B 113       3.265 -60.184 -36.429  1.00 19.49       C
ATOM    296  C   LEU B 113       2.040 -60.521 -37.274  1.00 18.73       C
ATOM    297  O   LEU B 113       2.143 -61.252 -38.255  1.00 18.44       O
ATOM    298  CB  LEU B 113       3.405 -61.198 -35.289  1.00 18.38       C
ATOM    299  CG  LEU B 113       4.777 -61.270 -34.605  1.00 20.59       C
ATOM    300  CD1 LEU B 113       4.656 -62.059 -33.311  1.00 20.01       C
ATOM    301  CD2 LEU B 113       5.794 -61.914 -35.538  1.00 20.23       C
ATOM    302  N   ALA B 114       0.875 -60.010 -36.892  1.00 18.96       N
ATOM    303  CA  ALA B 114      -0.334 -60.292 -37.661  1.00 18.70       C
ATOM    304  C   ALA B 114      -0.288 -59.578 -39.019  1.00 19.30       C
ATOM    305  O   ALA B 114      -0.602 -60.167 -40.052  1.00 20.62       O
ATOM    306  CB  ALA B 114      -1.562 -59.855 -36.889  1.00 16.45       C
ATOM    307  N   ALA B 115       0.082 -58.303 -39.000  1.00 20.57       N
ATOM    308  CA  ALA B 115       0.167 -57.516 -40.229  1.00 21.84       C
ATOM    309  C   ALA B 115       1.140 -58.192 -41.189  1.00 21.58       C
ATOM    310  O   ALA B 115       0.815 -58.464 -42.345  1.00 22.14       O
ATOM    311  CB  ALA B 115       0.636 -56.108 -39.911  1.00 19.85       C
ATOM    312  N   TRP B 116       2.334 -58.476 -40.688  1.00 22.12       N
ATOM    313  CA  TRP B 116       3.365 -59.126 -41.478  1.00 23.22       C
ATOM    314  C   TRP B 116       2.871 -60.434 -42.123  1.00 23.55       C
ATOM    315  O   TRP B 116       3.048 -60.643 -43.329  1.00 22.19       O
ATOM    316  CB  TRP B 116       4.584 -59.367 -40.579  1.00 26.08       C
ATOM    317  CG  TRP B 116       5.699 -60.136 -41.204  1.00 27.40       C
ATOM    318  CD1 TRP B 116       6.473 -59.761 -42.271  1.00 28.30       C
ATOM    319  CD2 TRP B 116       6.168 -61.418 -40.793  1.00 28.77       C
ATOM    320  NE1 TRP B 116       7.401 -60.742 -42.547  1.00 29.04       N
ATOM    321  CE2 TRP B 116       7.234 -61.771 -41.655  1.00 30.37       C
ATOM    322  CE3 TRP B 116       5.794 -62.308 -39.778  1.00 30.49       C
ATOM    323  CZ2 TRP B 116       7.929 -62.981 -41.529  1.00 31.08       C
ATOM    324  CZ3 TRP B 116       6.485 -63.510 -39.653  1.00 31.85       C
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ATOM    325  CH2 TRP B 116       7.541 -63.834 -40.527  1.00 32.27           C
ATOM    326  N   SER B 117       2.231 -61.304 -41.338  1.00 21.35           N
ATOM    327  CA  SER B 117       1.735 -62.573 -41.873  1.00 22.61           C
ATOM    328  C   SER B 117       0.665 -62.383 -42.940  1.00 23.56           C
ATOM    329  O   SER B 117       0.463 -63.262 -43.780  1.00 23.11           O
ATOM    330  CB  SER B 117       1.167 -63.462 -40.756  1.00 20.72           C
ATOM    331  OG  SER B 117       0.010 -62.889 -40.169  1.00 22.72           O
ATOM    332  N   LEU B 133      11.788 -52.846 -25.860  1.00 23.38           N
ATOM    333  CA  LEU B 133      11.903 -54.293 -26.020  1.00 24.54           C
ATOM    334  C   LEU B 133      11.209 -54.833 -27.276  1.00 22.84           C
ATOM    335  O   LEU B 133      11.784 -55.619 -28.027  1.00 21.86           O
ATOM    336  CB  LEU B 133      11.328 -54.996 -24.786  1.00 25.48           C
ATOM    337  CG  LEU B 133      11.388 -56.527 -24.780  1.00 27.50           C
ATOM    338  CD1 LEU B 133      12.840 -56.984 -24.866  1.00 28.69           C
ATOM    339  CD2 LEU B 133      10.735 -57.059 -23.509  1.00 28.04           C
ATOM    340  N   THR B 134       9.975 -54.401 -27.499  1.00 21.72           N
ATOM    341  CA  THR B 134       9.202 -54.860 -28.639  1.00 21.22           C
ATOM    342  C   THR B 134       9.693 -54.326 -29.986  1.00 20.62           C
ATOM    343  O   THR B 134       9.843 -55.091 -30.932  1.00 20.33           O
ATOM    344  CB  THR B 134       7.716 -54.509 -28.449  1.00 20.99           C
ATOM    345  OG1 THR B 134       7.257 -55.075 -27.210  1.00 20.94           O
ATOM    346  CG2 THR B 134       6.872 -55.073 -29.600  1.00 20.64           C
ATOM   3608  N   LYS B 136      12.595 -53.366 -30.809  1.00 21.46           N
ATOM   3609  CA  LYS B 136      13.886 -53.949 -31.144  1.00 22.79           C
ATOM   3610  CB  LYS B 136      14.713 -54.196 -29.879  1.00 24.70           C
ATOM   3611  CG  LYS B 136      16.183 -54.424 -30.178  1.00 27.75           C
ATOM   3612  CD  LYS B 136      16.998 -54.494 -28.902  1.00 30.17           C
ATOM   3613  CE  LYS B 136      18.479 -54.671 -29.203  1.00 32.33           C
ATOM   3614  NZ  LYS B 136      19.278 -54.641 -27.944  1.00 33.37           N
ATOM   3615  C   LYS B 136      13.793 -55.229 -31.966  1.00 23.46           C
ATOM   3616  O   LYS B 136      14.561 -55.407 -32.912  1.00 23.71           O
ATOM    347  N   TRP B 137      12.868 -56.127 -31.633  1.00 21.78           N
ATOM    348  CA  TRP B 137      12.753 -57.345 -32.424  1.00 22.06           C
ATOM    349  C   TRP B 137      11.768 -57.202 -33.574  1.00 21.75           C
ATOM    350  O   TRP B 137      11.936 -57.822 -34.623  1.00 21.76           O
ATOM    351  CB  TRP B 137      12.361 -58.552 -31.553  1.00 21.20           C
ATOM    352  CG  TRP B 137      10.990 -58.525 -30.922  1.00 20.23           C
ATOM    353  CD1 TRP B 137      10.696 -58.231 -29.618  1.00 19.62           C
ATOM    354  CD2 TRP B 137       9.748 -58.877 -31.544  1.00 18.68           C
ATOM    355  NE1 TRP B 137       9.349 -58.385 -29.390  1.00 19.31           N
ATOM    356  CE2 TRP B 137       8.743 -58.780 -30.555  1.00 18.97           C
ATOM    357  CE3 TRP B 137       9.383 -59.270 -32.840  1.00 19.75           C
ATOM    358  CZ2 TRP B 137       7.401 -59.058 -30.821  1.00 18.18           C
ATOM    359  CZ3 TRP B 137       8.046 -59.549 -33.107  1.00 18.87           C
ATOM    360  CH2 TRP B 137       7.072 -59.440 -32.099  1.00 18.94           C
ATOM    361  N   LEU B 138      10.741 -56.381 -33.386  1.00 21.61           N
ATOM    362  CA  LEU B 138       9.744 -56.188 -34.431  1.00 23.15           C
ATOM    363  C   LEU B 138      10.384 -55.558 -35.676  1.00 23.07           C
ATOM    364  O   LEU B 138       9.958 -55.801 -36.809  1.00 22.68           O
ATOM    365  CB  LEU B 138       8.618 -55.305 -33.886  1.00 23.87           C
ATOM    366  CG  LEU B 138       7.312 -55.155 -34.664  1.00 26.48           C
ATOM    367  CD1 LEU B 138       6.672 -56.508 -34.915  1.00 25.34           C
ATOM    368  CD2 LEU B 138       6.383 -54.267 -33.851  1.00 25.90           C
ATOM   3644  N   LYS B 140      12.801 -56.332 -37.241  1.00 27.38           N
ATOM   3645  CA  LYS B 140      13.279 -57.337 -38.182  1.00 28.05           C
ATOM   3646  CB  LYS B 140      13.893 -58.501 -37.401  1.00 29.91           C
ATOM   3647  CG  LYS B 140      15.134 -58.057 -36.635  1.00 31.62           C
ATOM   3648  CD  LYS B 140      15.719 -59.149 -35.757  1.00 33.53           C
ATOM   3649  CE  LYS B 140      16.974 -58.634 -35.055  1.00 34.46           C
ATOM   3650  NZ  LYS B 140      17.692 -59.713 -34.320  1.00 36.17           N
ATOM   3651  C   LYS B 140      12.254 -57.833 -39.212  1.00 27.83           C
ATOM   3652  O   LYS B 140      12.602 -58.562 -40.142  1.00 27.80           O
ATOM    369  N   ILE B 141      10.992 -57.445 -39.052  1.00 26.40           N
ATOM    370  CA  ILE B 141       9.963 -57.818 -40.016  1.00 26.09           C
ATOM    371  C   ILE B 141       9.316 -56.542 -40.530  1.00 25.81           C
ATOM    372  O   ILE B 141       8.353 -56.586 -41.305  1.00 26.10           O
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ATOM     373  CB   ILE B 141      8.854  -58.721  -39.405  1.00  26.39       C
ATOM     374  CG1  ILE B 141      8.298  -58.092  -38.127  1.00  26.45       C
ATOM     375  CG2  ILE B 141      9.401  -60.118  -39.145  1.00  28.33       C
ATOM     376  CD1  ILE B 141      7.136  -58.845  -37.549  1.00  26.95       C
         TER
```

The following examples are presented for purposes of illustration only and are not intended to limit the scope of the invention in any way.

EXAMPLE 1

This example describes the crystallization of the *E. coli* MurG protein and the determination of the coordinates of the three-dimensional crystal structure. This example also describes the identification of the donor nucleotide binding site, the acceptor binding site and the membrane association site of the MurG protein.

Abstract

The 1.9 Å X-ray structure of a membrane-associated glycosyltransferase involved in peptidoglycan biosynthesis is reported. This enzyme, MurG, contains two ?/? open sheet domains separated by a deep cleft. The C-terminal domain contains the UDP-GlcNAc binding site while the N-terminal domain contains the acceptor binding site and likely membrane association site. Combined with sequence data from other MurG homologs, this structure provides insight into the residues that are important in substrate binding and catalysis. We have also noted that a conserved region found in many UDP-sugar transferases maps to a ?/?/?/? supersecondary structural motif in the donor binding region of MurG, an observation that is be helpful in glycosyltransferase structure prediction.

Methods

Crystallization

E. coli MurG containing a C-terminal LEHHHHHH sequence was purified as described(Ha *et al.*, 1999) and concentrated to 10 mg ml^{-1} in 20 mM Tris-HCl, pH 7.9/ 150 mM NaCl/ 50 mM EDTA. The protein concentrate was mixed with UDP-GlcNAc

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in a 1:3 molar ratio. Crystals were grown at room temperature using the hanging-drop vapor-diffusion method by mixing equal volumes of protein with reservoir solution (0.1 M NaMES, pH 6.5/ 0.96 M $(NH_4)_2SO_4$/ 0.4% Triton X-100/ 10 mM DTT). Triclinic crystals with a typical size of 0.2 mm X 0.1 mm X 0.1 mm grew within a week. The crystals belong to the P1 space group, with two molecules per asymmetric unit. The cell dimensions are a=60.613 Å, b=66.356 Å, c=67.902 Å, ?=64.294, ?=83.520, ?????????????

Data collection and processing

All data sets were collected at 100 K on previously flash frozen crystals. Crystals were equilibrated in a cryoprotectant buffer with 0.1 M NaMES, pH 6.5, 1.44 M $(NH_4)_2SO_4$, 0.4% Triton X-100, and 20% glycerol. Heavy-atom soaks were carried out in the same buffer containing one of the following heavy-atom solutions: 2 mM $HgCl_2$, 1 mM $(NH_4)_2WS_4$, 1 mM $(NH_4)_2OsBr_6$. Crystals were flash-frozen in liquid nitrogen. $HgCl_2$ (form A derivative) and $(NH_4)_2OsBr_6$ derivative data were collected at an R-AXISIIC imaging plate detector mounted on a Rigaku 200HB generator. Native, $HgCl_2$ (form B derivative), and $(NH_4)_2WS_4$ derivative diffraction data were collected at beam-line BioCARS-14B at the Advanced Photon Source, at wavelengths 1.0092 Å, 0.9900 Å and 1.2147 Å respectively. Collection of data on the $HgCl_2$ derivative was initially designed for MAD phasing; however, the mercury derivative proved to be unstable to X-rays, and after a two-hour exposure to synchrotron radiation the form A derivative metamorphosed into a different mercury derivative (form B) that was suitable for MIR phasing. All the data were reduced using DENZO and SCALEPACK (Otwinowski & Minor, 1997), and processed with CCP4 programs (CCP4, 1994).

Structure determination and refinement

The structure was solved by multiple isomorphous replacement combined with anomalous scattering of mercuric derivatives (Table 1). Initial MIR phases calculated with program MLPHARE had a mean figure of merit of 0.44 to 2.5 Å, and were improved by solvent flattening and histogram matching using DM. An MIR map was generated which had continuous electron density for most regions of the protein. A model was built with the program O (Jones *et al.*, 1991), and the structure was refined against 1.9 Å data using energy minimization, simulated annealing and B-factor

refinement with the program CNS (Brunger *et al.*, 1998). The N-terminal six residues and the C-terminal His-tag had no electron density and were not included in this model. There was no electron density for UDP-GlcNAc.

Results and discussion

Overall fold

The crystal structure of *E. coli* MurG was solved by a combination of multiple isomorphous replacement and anomalous scattering, and refined to 1.9 Å resolution (Table 1).

Table 1. Summary of crystallographic and refinement data

Data set	Native	HgCl$_2$ (form A derivative)	HgCl$_2$ (form B derivative)	(NH$_4$)$_2$WS$_4$	(NH$_4$)$_2$OsBr$_6$
Resolution (Å)	1.9	2.0	1.9	2.4	2.3
Observations	288,150	101,913	245,320	44,366	106,606
Unique reflections	65,567	53,391	65,581	27,950	36,443
R$_{sym}$[1](last shell)	0.032 (0.187)	0.043 (0.200)	0.042 (0.296)	0.031 (0.080)	0.056 (0.302)
I/? (last shell)	41.9 (7.0)	20.4 (2.9)	29.0 (3.7)	24.6 (8.2)	19 6 (2.5)
Completeness (last shell)	97.7% (96.4%)	91.4% (66.6%)	97.4% (94.0%)	83.8% (62.0%)	94.3% (78.6%)
MIR analysis (40.0 - 2.5 Å)					
Mean isomorphous difference[2]		0.163	0.130	0.068	0.134
Phasing power[3](last shell)		1.09 (0.73)	0.57 (0.50)	0.61 (0.24)	0.61 (0.58)
R$_{cullis}$ [4](last shell)		0.81 (0.91)	0.94 (0.96)	0.92 (0.99)	0.94 (0.95)
Anomalous R$_{cullis}$ [4](last shell)		0.96 (1.00)	0.95 (1.00)		

Refinement statistics				
Resolution	40.0 - 1.9 Å		R. m. s. d.[7]	
Reflections (|F| > 2?)	61,989		Bonds (Å)	0.006
Protein atoms (a. u.)	5,280		Angles (°)	1.29
Water Atoms	298			
Sulfate groups	1		Ramachandran plot[8]	
R-factor[5]	22.0%		Residues in most favored region	94.6%
R-free[6]	24.7%		Residues in additional allowed region	5.4%

[1]R$_{sym}$ = ?| I$_i$ - <I> | / ?I$_i$, where I$_i$ is the intensity of a reflection, and <I> is the average intensity of that reflection.

[2]Mean isomorphous difference = ? |F$_{PH}$ - Fp| / ?F$_{PH}$, where F$_{PH}$ and Fp are the derivative and native structure factors respectively

[3]Phasing power is the ratio of the mean calculated derivative structure factor to the mean lack of closure error.

[4]R$_{cullis}$ is the mean residual lack of closure error divided by the dispersive or anomalous difference.

[5]R-factor = ? | |F$_{obs}$| - |F$_{calc}$| | / ? |F$_{obs}$|

[6]R-free is the R-factor calculated using 10% of the reflection data chosen randomly and omitted from the start of refinement.

[7]R. m. s. d., root-mean-square deviations from ideal bond lengths and bond angles.

[8]Calculated with program PROCHECK.

The structure consists of two domains separated by a deep cleft (Fig. 2a). Both domains exhibit an ?/? open-sheet structure and have high structural homology despite minimal sequence homology (RMSD = 2.02 over 85 aligned C? atoms). The N-domain includes residues 7-163 and 341-357, and contains seven parallel ?-strands and six ?-helices, the last of which originates in the C-domain (Fig. 2b). The C-domain comprises residues 164-340 and contains six parallel ?-strands and eight ?-helices, including one irregular bipartite helix (?-link) that connects the N-domain to the first ?-strand of the C-domain. The ?-strands in both domains are ordered as for a typical Rossman fold. The N- and C-domains are joined by a short linker between the seventh ?-strand of the N-domain and the ?-link of the C-domain. This inter-domain linker and the peptide segment that joins the last helix of the C-domain to the last helix of the N-domain define the floor of the cleft between the two domains. The cleft itself is about 20 Å deep and 18 Å across at its widest point. Contacts < 4 Å across the cleft are limited primarily to interactions between residues from C-?5 to the loop connecting N-?5 to N-?5.

The ?/? open-sheet motif (Rossman fold) adopted by both the N- and C-domains of MurG is characteristic of domains that bind nucleotides (Branden & Tooze, 1998). Classical Rossman domains typically contain at least one conserved glycine rich motif, with the consensus sequence GXGXXG, located at a turn between the carboxyl end of one ?-strand and the amino terminus of the adjacent ?-helix (Baker et al., 1992). This motif is involved in binding the negatively charged phosphates (Carugo & Argos, 1997). There are three glycine rich loops (G loops) in E. coli MurG (Fig. 3a) that may be variants on the phosphate binding loops found in other dinucleotide binding proteins (see below).

Sequence homology

Amino acid sequences for eighteen MurG homologs are now available. The sequence similarity between E. coli MurG and homologs from other bacterial strains ranges from less than 30% to more than 90% depending on the evolutionary relationship between the organisms. In all MurG homologs, however, there are several invariant residues. Fig. 3a shows a sequence alignment for a subset of MurG homologs with the invariant and

highly conserved residues indicated. These residues, which include the three G loops, have been highlighted in the *E. coli* MurG structure (Fig. 3b). Almost all of the invariant residues are located at or near the cleft between the two domains. Two of the G loops are found in the N domain (between N-?1/N-?1 and N-?4/N-?4) and one is found in the C-domain (between C-?1/C-?1). The strict conservation of the highlighted residues among different bacterial strains, and their location as determined from the *E. coli* MurG structure, implicates them in substrate binding and catalytic activity.

Structural homology reveals the donor binding site

The three-dimensional backbone structure of *E. coli* MurG was compared to known protein structures, including the three other NDP-glycosyltransferase structures that have been reported (Charnok & Davies, 1999; Gastinel *et al.*, 1999; Vrielink *et al.*, 1994). The C-terminal domain was found to have significant structural homology (RMSD= 2.218 Å for 89 aligned C? atoms) to the C-terminal domain of phage T4 ?-glucosyltransferase (BGT), an enzyme that catalyzes the glucosylation of hydroxymethyl-cytosines in duplex DNA. A co-crystal structure of BGT with UDP bound in the C-terminal domain reveals the topology of the UDP binding pocket and also shows important contacts to the nucleotide (Moréra *et al.*, 1999; Vrielink *et al.*, 1994). These contacts include: a) hydrogen bonds from the backbone amide of I238 to the N3 and O4 positions of the base; b) hydrogen bonds between the carboxyl side chain of E272 and the O2' and O3' hydroxyls of the ribose ring; and c) contacts from a GGS motif in the loop following the first ?-strand of the C domain to the alpha phosphate of UDP. The structurally homologous C-domain of MurG contains a topologically similar pocket (Fig. 4a). Furthermore, even though the two domains share only 11% sequence identity overall, there are identical residues in the same spatial location in *E. coli* MurG and in BGT. Based on this comparison, we have concluded that the C-domain of *E. coli* MurG is the UDP-GlcNAc binding site.

We have docked UDP-GlcNAc into the C-domain of *E. coli* MurG using the information on how UDP binds to BGT as a guide. As shown in Figure 4b, the uracil is held in place by contacts from the N3 and O4 atoms to the backbone amide of I245. The O2' and O3' hydroxyls on the ribose sugar are within hydrogen bonding distance of the invariant glutamate residue (E269) in the middle of helix C-?4. The conserved GGS

motif in G loop 3 is positioned to contact the alpha phosphate. When these contacts are made, the UDP-GlcNAc substrate fits nicely into a pocket in the C-domain, where it is surrounded by many of the invariant residues identified through sequence analysis of other MurG homologs. It is possible to propose roles for some of these invariant residues from the model. For example, the side chain of R261 can be rotated to contact the second phosphate; this contact may help explain why UDP binds significantly better to MurG than UMP. We propose that R261 plays an important role in catalysis by stabilizing the UDP leaving group via electrostatic interactions. The side chain of Q289 is within hydrogen bonding distance of the C4 hydroxyl of the GlcNAc sugar. This contact may explain why MurG can discriminate between UDP-GlcNAc and its C4 axial isomer, UDP-GalNAc (Ha *et al.*, 1999).

The acceptor binding site

Structural considerations suggest that the primary acceptor binding site is located in the N-terminal domain of MurG. This domain contains three highly conserved regions, two of which are glycine-rich loops that face the cleft (Fig 3a and 4c). These G loops are reminiscent of the phosphate binding loops found in other nucleotide binding proteins, and are most likely involved in binding to the diphosphate on Lipid I. The N-termini of the helices following each G loop form opposite walls of a small pocket between the G loops. The helix dipoles create a positively charged electrostatic field in the pocket that can stabilize the negative charged diphosphates. When the diphosphate of the acceptor is anchored in the pocket created by the G-loops, the MurNAc sugar emerges into the cleft between domains and the C4 hydroxyl can be directed towards the anomeric carbon of the GlcNAc for attack on the face opposite the UDP leaving group. The third conserved region in the N domain spans the loop from the end of N-?5 to the middle of N-?5. Kinetic analysis of mutants is required to evaluate the roles of these residues (Ha *et al.*, 1999; Men *et al.*, 1998).

Proposed membrane association site

MurG associates with the cytoplasmic surface of bacterial membranes where it couples a soluble donor sugar to the membrane anchored acceptor sugar, Lipid I. Analysis of the *E. coli* MurG structure shows that there is a hydrophobic patch consisting of residues

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I75, L79, F82, W85 and W116 in the N-domain, which is surrounded by basic residues (K72, K140, K69, R80, R86, R89). We propose that this is the membrane association site and that association involves both hydrophobic and electrostatic interactions with the negatively charged bacterial membrane. The location of this patch in MurG is also consistent with the proposed acceptor binding site: membrane association at this patch would bring the two N-terminal G loops close to the membrane surface where the diphosphate portion of the acceptor is located (Fig. 4c). Moreover, the cleft between the two domains would remain accessible, consistent with the biochemical requirement that the soluble UDP-GlcNAc donor be able to find its binding site from the cytoplasm.

Implications for other glycosyltransferases

Glycosyltransferases that utilize an activated nucleotide sugar as a donor comprise a large family of enzymes in both prokaryotes and eukaryotes, and they play central roles in many important biological processes (Dennis et al., 1999; Koya et al., 1999; Verbert & Cacan, 1999). Glycosyltransferases are typically classified according to the nucleotide sugar they utilize, and it has frequently been noted that there is no significant sequence homology even among glycosyltransferases in the same family. This has made it difficult to identify common structural features and residues important in binding and catalysis. There are only three other glycosyltransferase structures available, and although none of them shows any sequence homology to MurG, a structural comparison indicates that one of them, BGT, contains a related donor binding site.

In addition to this structural homology, we have identified a strikingly similar sequence motif in the MurG family and certain other UDP-glycosyltransferase families. This sequence motif spans about a thirty amino acid stretch in the C-domain of MurG and includes most of the invariant residues found in that domain. As shown in Figure 3a, a similar motif is found in the UDP-glucuronosyltransferases (Mackenzie, 1990). Certain residues are identical, including a number of prolines and glycines, and the spacing between them is invariant. This suggests that the UDP-glucuronosyltransferases contain a region of ?/? supersecondary structure that is involved in a similar function as the corresponding region in MurG (Fig. 3c). This region binds the donor sugar. By analyzing the similarities and differences between the conserved residues in this subdomain in the MurG family and other UDP-glycosyltransferase families, it may be

possible to identify – and perhaps alter - residues that are involved in determining donor selectivity. We note that it would be useful to be able to manipulate donor specificity because it would extend the utility of glycosyltransferases as reagents for glycosylation of complex molecules. Altered glycosyltransferases could also be useful for remodeling cell surfaces and for probing the biological roles of particular carbohydrate structures.

Conclusion

This first structure of a member of the MurG family of glycosyltransferases lays the groundwork for further mechanistic and structural investigations, which may lead to the design of inhibitors and perhaps even new antibiotics. The work also shows that there can be conserved subdomains even in very different glycosyltransferase families. Information on conserved subdomains will be useful for structure prediction and may help guide experiments directed towards changing substrate specificity.

EXAMPLE 2

This example describes a method of isolating the C-terminal domain of the *E. coli* MurG protein, expressing the domain in *E. coli* cells and utilizing nuclear magnetic resonance (NMR) to determine the ability of compounds to bind.

MurG can also be used to determine the ability of a chemical compound to bind to the C domain by a) determining the start of c domain based on the MurG crystal structure; b) independently expressing the C domain; and c) using NMR methods to identify binding site and/or bound conformation of ligand. The same procedure is used for the acceptor binding domains.

NMR methods are used to identify the protein binding sites nad screen for ligands that bind. The MurG C-terminal domain region of the protein has been expressed independently. The C domain has a much lower molecular weight than the full-length protein. Therefore, the expression of the C domain results in much sharper NMR peaks which will facilitate the NMR interpretation. Also the protin chemical shifts are very sensitive to their environment. Binding of a compound will introduce local environment changes, thus changing the proton chemical shifts. In this way, residues involved in the binding can be differentiated easily from other amino acid residues not involved in

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binding a ligand. This method has also been used to identify ligands that bind to low molecular weight drug targets (i.e., small proteins).

Relevant references to NMR techniques are: Discovering high-affinity ligands for proteins: SAR by NMR, S. Shuker, P. Hajduk, R. Meadows, and S. Fesik, Science 274, 1531 (1996); Lin Y, Nageswara Rao BD. Structural characterization of adenine nucleotides bound to Escherichia coli adenylate kinase. 1. Adenosineconformations by proton two-dimensional transferred nuclear Overhauser effect spectroscopy. Biochemistry. 2000 Apr 4;39(13):3636-46; and Fejzo J, et al., Chem Biol 1999 Oct;6(10):755-69 (incorporated herein by reference).

The SHAPES strategy is also useful for NMR identification of binding residues, ligands and drug discover which is an NMR-based approach for lead generation in drug discovery. Recently, it has been shown that nuclear magnetic resonance (NMR) may be used to identify ligands that bind to low molecular weight protein drugtargets. Recognizing the utility of NMR as a very sensitive method for detecting binding, we have focused on developing alternative approaches that are applicable to larger molecular weight drug targets and do not require isotopic labeling. A new method for lead generation (SHAPES) uses NMR to detect the binding of a limited but diverse library of small molecules to a potential drug target. The compound scaffolds are derived from shapes most commonly found in known therapeutic agents. NMR detection of low (microM-mM) affinity binding is achieved using either differential line broadening or transferred NOE (nuclear Overhauser effect) NMR techniques. The SHAPES method for lead generation by NMR is useful for identifying potential lead classes of drugs early in a drug design program, and is easily integrated with other discovery tools such as virtual screening, high-throughput screening and combinatorial chemistry.

EXAMPLE 3

This example describes the method of using the three-dimensional structure of *E. coli* MurG to determine the crystal structures of its mutant, enzyme-ligand complex, and MurG homologs, which share the same folding motif.

First, a crystalline form of the new protein or the protein complex should be obtained. The E.coli MurG mutants should crystallized in a condition very similar to

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what we have showed in the method section. The protein-ligand complex can be obtained by soaking the protein crystals in a ligand-containing buffer. Other MurG homologs can be expressed in a His-tagged fashion and purified using affinity colume. Presumably they can be crystallized in a similar way using a detergent as the additive. Next, the diffraction data should be collected and processed. After the data collection, the molecular replacement method is used to determine the unknown structure. Either the whole E. coli MurG protein or one single domain can serve as a search model. This search model can be rotated and translated until the correct orientation is located in the unit cell of this unknown structure. The search model may only represent part of the contents of the asymmetric unit. However, the location of the first model is now already available. While the first location of the search model is fixed, the second round of translation search can be carried out to search more molecules or domains in the asymmetric unit cell. The phases from the final model generated by molecular replacement can be used to calculate the electron density map. Finally, a model is built based on the electron density map, and the model needs to be refined using program CNS or XPLOR.

EXAMPLE 4

This example describes the method of using the three-dimensional coordinate structure of E. coli MurG to produce a protein fragment that can be used in an NMR-based lead discovery program. The crystal structure reveals the boundaries of the C domain and permits us to design a gene containing only the C domain from the gene containing both domains. The C domain starting at residue 164 and ending at residue 340 was cloned into an expression vector to generate a C-terminal His tag fusion. It was over-expressed in E. coli cells and purified by affinity colume. The protein was shown to be monomeric by size exclusion chromatography and to be soluble at least up to 0.15 mM, a concentration more than adequate for NMR analysis. C domains from other Murg homologues can be similarly expressed and used.

EXAMPLE 5

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This example describes the co-crystallization of a MurG protein with a ligand. A MurG-ligand complex is formed by either co-crystallizing MurG protein with appropriate ligand or soaking the MurG crystals in buffers containing appropriate ligand. Co-crystallization is done by pre-mixing the protein sample with a certain amount of substrate or substrate analogs. Then the hanging drop method is used to produce crystals as described infra.

Alternatively, ligans are incorporated into the crystals by soaking the protein crystals in the ligand containing buffer for a period of time to allow for infiltration into the crystal. The time ranges from a couple of hours to a couple of days. The concentration of ligand in the buffer ranges from several milimolar to several hundred mili molar.

DEPOSIT OF COORDINATES

The crystal structure three-dimensional coordinates of the *E. coli* MurG as set forth in Table 1 were deposited with the Protein Data Bank and have been assigned the indicated ID Code (Accession No.) 1F0K.

Although the invention is described in detail with reference to specific embodiments thereof, it will be understood that variations which are functionally equivalent are within the scope of this invention. Indeed, various modifications of the invention in addition to those shown and described herein will become apparent to those skilled in the art from the foregoing description and accompanying drawings. Such modifications are intended to fall within the scope of the appended claims.

Various publications are cited herein, the disclosures of which are incorporated by reference in their entireties.

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